SAC/SAC-CI Program Combined with Gaussian for Calculating Ground, Excited, Ionized, and Electron-Attached States and Singlet, Doublet, Triplet, Quartet, Quintet, Sextet, and Septet Spin States and Their Analytical Energy Gradients

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Part I. Overview of SAC/SAC-CI Gaussian Version Program

I-A. Introduction

This program calculates the followings.

1. SAC (Symmetry-Adapted-Cluster) single-double(SD-*S*) wave function for singlet closed-shell system.
2. SAC-CI SD-*R* and general-*R* wave functions for the ground and excited states of
   singlet states,
   triplet states,
   doublet ionized states,
   doublet electron attached (anionized) states,
   quartet (ionized) states,
   quintet states,
   sextet (ionized) states, and
   septet states.

   In the SAC-CI SD-*R* method, the linked operators consists of the single and double excitation operators, while in the general-*R* method, higher excitation operators up to sextuple excitations are also included. The SAC-CI SD-*R* method is suitable for ordinary one-electron processes like excitations and ionizations, while the SAC-CI general-*R* method is useful for studying multi-electron processes such as two- three-electron excitation processes and shake-up ionizations. (See Sec. I-C for more details.)
3. Analytical energy gradients and optimized geometries for the ground and excited states calculated by the SAC/SAC-CI method for
   singlet state,
   triplet state,
   doublet ionized state,
   doublet electron-attached (anionized) state,
   quartet (ionized) states,
   quintet states,
   sextet (ionized) states, and
   septet states.
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5. Density and spin density matrices for the above states.
6. Transition densities and transition moments among the above SAC/SAC-CI states.
7. One-electron properties for the above states.
8. Circular dichroism (CD) of optically active molecules.
9. Hyperfine splitting constants of open-shell molecules.
10. Detailed explanation of each step of the SAC/SAC-CI program is found in Part II of this guide.

Remarks

(1) The excitation operators in the SAC method are denoted by S or s and those in the SAC-CI method by R or r (refs. c-1-5).
(2) When the weight of the Hartree-Fock configuration is small, we recommend to use EGCI and GWF/EX-EGWF (including MR-SAC) methods instead of the SAC/SAC-CI method. (See refs. c-7-10.)
(3) The SAC/SAC-CI SD-*R* part of this program is based on SAC85 program (refs. b-1,2) and modified for larger-scale, more speedy calculations. The SAC-CI general-*R* and high-spin part is a simplified version of the more general EGWF/EX-EGWF program (ref. b-3).

Input Method

SAC-CI/Gaussian input are done with Keyword Input which are explained in the corresponding links of Users Reference. More detailed Keyword Input that provides more flexible input is also available and are given in Part I-H of this guide. The most flexible input was done by the Namelist input, though it is now somewhat old, and its account is given below at the beginning of the Link 923 SAC/SAC-CI code. More details are given in Part II of this guide.

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I-C. Brief explanation of the SAC/SAC-CI method

I-C-1. SAC method for ground state

For the totally symmetric singlet closed-shell state, we define symmetry adapted cluster (SAC) expansion as,

$$\left|\Psi_g\right\rangle = \exp(\sum_I C_I S_I)\left|0\right\rangle$$

$$= (1 + \sum_I C_I S_I + \frac{1}{2}\sum_{I,J} C_I C_J S_I S_J + \ldots)\left|0\right\rangle$$

where $\left|0\right\rangle$ is Hartree-Fock and S_I is symmetry adapted excitation operator.

We include in the linked terms S_I totally symmetric single and double excitation operators of the forms,

single excitation, S_i^a

double excitation, $S_i^a S_j^b$

where

$$S_i^a = 1/\sqrt{2}(a_{a\alpha}^\dagger a_{i\alpha} + a_{a\beta}^\dagger a_{i\beta})$$

and *i*, *j* are occupied MOs and *a*, *b* are unoccupied MOs. For the unlinked operators $S_I S_J$, the products of the double excitation operators, which are quadruple excitation operators,

quadruple excitation, $S(2)S(2) : S_i^a S_j^b S_k^c S_l^d$

are included. Other unlinked operators of the forms,

$S(1)S(1)$, $S(1)S(1)S(1)$, $S(1)S(1)S(1)S(1)$,
$S(1)S(2)$, $S(1)S(1)S(2)$

are included by options (see 'FullUnlinked' and 'PlusULSAC' of the Keyword input and the explanation in step ULINT).

I-C-2. SAC-CI method for excited, ionized, and electron-attached states

The excited, ionized, and electron attached states are calculated by the SAC-CI method. We describe the electron correlations in the excited state on the basis of those in the ground state.

The SAC-CI wave function is written as,

$$\left|\Psi_e\right\rangle = \sum_K d_K \left|\Phi_K\right\rangle$$

$$= (\sum_K d_K R_K + \sum_{K,I} d_K C_I R_K S_I + ...)|0\rangle - \sum_K d_K S_{gK} |\Psi_g\rangle$$

where

$$S_{gK} = \langle \Psi_g | R_K | \Psi_g \rangle .$$

(A) SAC-CI SD-*R* Method

In the SAC-CI SD-*R* method for singlet to triplet states, R_K operators are restricted to single and double (SD) excitation operators as shown in the following table. S_0, identity operator may also be included for the singlet state (see WITHHF in step SCIV, SCINV, DAS, and DNAS).

Table. Linked R_K operators in the SD-*R* method

	Single	Double
Singlet excitation	S_i^a	$S_i^a S_j^b$
Triplet excitation	T_i^a	$T_i^a S_j^b$
Ionization (doublet)	I_i	$I_i S_j^a$
Electron attachment (doublet)	A^a	$A_a S_i^b$

$T_i^a = a_{a\alpha}^\dagger a_{i\beta}$, $I_i = a_{i\beta}$, $A^a = a_{a\alpha}^\dagger$

For the unlinked operators, $R_K S_I$, we include

single R_K * double S_I = triple excitation

and

double R_K * double S_I = quadruple excitation.

For single electron processes such as ordinary excitations and ionizations, the second unlinked operators are less important and so can be omitted by the keyword, WithoutR2S2, for saving computational time.

Other unlinked operators of the forms,

$$R(1)S(1),\ R(1)S(1)S(1),\ R(1)S(1)S(1)S(1),\ R(1)S(1)S(2),$$
$$R(2)S(1),\ R(2)S(1)S(1)$$

are included by options (see 'FullUnlinked' and 'PlusULSACCI' of the Keyword input and the explanation in step ULINT).

In the SAC-CI high-spin part for quartet to septet spin states, the lowest SAC-CI excitation operators are two-electron excitation operators for quartet and quintet multiplicities and three-electron excitation operators for sextet and septet spin multiplicities. Following table shows the linked operators for the quartet to septet-spin multiplet states.

Table. Linked R_K operator for the high-spin SAC-CI

Quartet	R_{ij}^{a}	$R_{ij}^{a}S_{k}^{b}$
Quintet	R_{ij}^{ab}	$R_{ij}^{ab}S_{kl}$
Sextet	R_{ijk}^{ab}	$R_{ijk}^{ab}S_{l}^{c}$
Septet	R_{ijk}^{abc}	$R_{ijk}^{abc}S_{l}^{d}$

$R_{ij}^{a} = a_{a\alpha}^{\dagger} a_{i\beta} a_{j\beta}$, $R_{ij}^{ab} = a_{a\alpha}^{\dagger} a_{b\alpha}^{\dagger} a_{i\beta} a_{j\beta}$, etc.

(B) SAC-CI general-*R* method

For the multi-electron processes, we have to choose R_K operators to include not only single and double excitation operators, but also triple-, quadruple-, and higher-excitation operators. This is done in the SAC-CI general-*R* part. In the present code, 1-6 excitation operators can be included in R_K. (For details, see ref. d-(22).)

I-C-3. Technical details - Selections of linked and unlinked operators

(A) SAC

The SAC wave function is given by

$$\left|\Psi_g\right\rangle = (1 + \sum_I C_I S_I + \frac{1}{2}\sum_{I,J} C_I C_J S_I S_J + \ldots)\left|0\right\rangle$$

The following approximation can be introduced for reducing computational time.

1) Selection of linked operators

(a) single excitation operators are included without selection.

(b) Double excitation operator, $S_i^a S_j^b$ is included when its second-order contribution to the energy is larger than a given threshold λ_g, i.e.,

$$|E_s| \geq \lambda_g$$

where

$$E_s = \frac{|H_{0s}|^2}{H_{ss} - H_{00}}$$

with

$$H_{0s} = \left\langle 0 \middle| H \middle| \Phi_s \right\rangle,\ H_{ss} = \left\langle \Phi_s \middle| H \middle| \Phi_s \right\rangle,\ H_{00} = \left\langle \Phi_0 \middle| H \middle| \Phi_0 \right\rangle \text{ and } \left|\Phi_s\right\rangle = S_i^a S_j^b \left|0\right\rangle.$$

(c) In Keyword Input

For SAC, λ_g is automatically set by the keywords, 'LevelOne/LevelTwo/LevelThree'.

Default value is 1.0×10^{-6} (LevelThree) and others are 5.0×10^{-6} (LevelTwo) and 1.0×10^{-5} (LevelOne). This threshold can be input with 'EThreS2'.

2) Selection of unlinked term, $C_I C_J S_I S_J \left|0\right\rangle$

For unlinked terms, we include the products of the linked operators whose SDCI coefficients *C* satisfy,

$$C \geq \tau_g .$$

Default value of τ_g is 5.0×10^{-3}. This threshold can be input with 'CThreULS2G'.

(B) SAC-CI

The SAC-CI wave function is written as

$$\left|\Psi_e\right\rangle = (\sum_K d_K R_K + \sum_{K,I} d_K C_I R_K S_I + ...)\left|0\right\rangle - \sum_K d_K S_{gK} \left|\Psi_g\right\rangle .$$

The perturbation selection can be done to reduce computational time.

1) Selection of linked operators

(a) All single excitation operators are included without selection.
(b) Double excitation operators are selected in the following way.

We are interested in *N* excited states and let $\psi(p)$ be primary reference states representing such *N* states

$$\psi(p) = \sum_i c_i(p)\varphi_i(p) \qquad (p=1,...,N)$$

which are obtained by a SECI, small SDCI, or small EGCI calculations. Three perturbation selection schemes are possible.

(b-1) Recommended (default)
We denote sample doubly excited (in SD-*R* method) or higher excited (in general-*R* method) configuration to be selected as ψ_s and define

$$E_s(p) = \frac{|H_s(p)|^2}{E(p) - H_{ss}}$$

where

$$H_s(p) = \left\langle \psi(p) \middle| H \middle| \psi_s \right\rangle, \quad E(p) = \left\langle \psi(p) \middle| H \middle| \psi(p) \right\rangle, \; H_{ss} = \left\langle \psi_s \middle| H \middle| \psi_s \right\rangle .$$

Now, in the selection, we include only such ψ_s which satisfies

$$|E_s(p)| \geq \lambda_e,$$

with at least one of the reference states $\psi(p)$. Default value of λ_e for SAC-CI is given by $\lambda_e = 1.0 \times 10^{-7}$ (LevelThree) and by 5.0×10^{-7} (LevelTwo) and 1.0×10^{-6} (LevelOne). λ_e can also be input by 'EThreR2'.

Other two selections schemes (non-default) are also possible (if you request so by Input).

(b-2) Old version ('LinkedSelection'=2)

Using $\varphi_i(p)$ (as main reference configurations) whose coefficients $c_i(p)$ are larger than 0.1 (see 'CThreMainConfig'),

$$E_{si}(p) = \frac{|H_{si}(p)|^2}{(H_{ii}(p) - H_{ss})}$$

where

$$H_{si}(p) = \langle \psi_s | H | \varphi_i(p) \rangle, \quad H_{ii}(p) = \langle \varphi_i(p) | H | \varphi_i(p) \rangle, \; H_{ss}(p) = \langle \psi_s | H | \psi_s \rangle.$$

Then, we include only such ψ_s which satisfies

$$|E_{si}(p)| \geq \lambda_e.$$

(b-3) Second old version ('LinkedSelection'=1)

We include only such ψ_s which satisfies

$$|c_i(p)|^2 |E_{si}(p)| \geq \lambda_e'$$

which takes the weight of the main reference configuration into account and the default of λ_e' is

$$\lambda_e' = 0.1 \times c_i(p)^2 \lambda_g.$$

2) Selection of unlinked terms,

In the unlinked term, $\sum_I d_K C_I R_K S_I$, we include all the double excitation operators S_I by default and important R_K operators whose SECI or SDCI coefficients D_K are $D_K \geq \tau_e$ Default of τ_e is 0.05. These values can be input by 'CThreULS2E', 'CThreULR1' and 'CThreULR2'.

(C) Direct algorism (G09.B01)

The direct SAC-CI code has been developed for the SAC/SAC-CI (SD-R) calculations for singlet, triplet, cation doublet, and anion doublet states and their analytical energy gradients. This new algorithm is more efficient than the conventional non-direct algorithm for large systems in

particular. The direct SAC-CI code does not apply to the general-R calculations.

In the direct SAC-CI code, the sigma-vector is directly generated in a similar way to the existing direct CI-like algorithms, but we can do perturbation selection of linked operators, which is important for dealing with large molecular systems.

The direct SAC-CI algorithm improves not only the efficiency but also the accuracy of the SAC-CI calculations, because the cut-off approximation in the unlinked terms is unnecessary there. For the SAC-CI SD-R calculations of singlet, triplet, cation doublet, and anion doublet states, we strongly recommend to use this direct method, although we retain the previous “non-direct” method as a default to maintain the consistency of our previous results.

I-D. Structure of the SAC/SAC-CI Gaussian version program

This program consists of SAC/SAC-CI SD-*R* part, SAC-CI general-*R* and high-spin part, and SAC/SAC-CI analytical energy gradient part for SD-*R*, general-*R*, and high-spin parts.

The SAC/SAC-CI SD-*R* part deals with the SAC/SAC-CI SD-*R* calculations for ground, excited, ionized, and electron-attached states with singlet, doublet, and triplet spin-multiplicities. The SAC-CI general-*R* part handles the SAC-CI general-*R* calculations for multi-electron processes (for details see ref. c-5) and the SAC-CI high-spin part (for details see ref. c-6) calculates quartet, quintet, sextet, and septet spin-multiplicities. The SAC-CI general-*R* calculations are possible for all spin-multiplicities, i.e., from singlet to septet multiplicities. The calculations of analytical gradients can be done essentially to all of the above parts, but readers may refer to I-D-5.

The structure of the program within the Gaussian suite of programs is shown below. L923 and the part of L801 (Minimum Orbital-Deformation (MOD) method and reordering MOs) and L1111 (SAC/SAC-CI derivatives) are developed by Nakatsuji Laboratory. Readers should also refer to User's Reference and Programmer's Reference.

Lxxxx denotes constituent programs called Link.

```
L1 (processing route section)
|
L101,L103 (reading molecular specification, geometry optimization)
|
L202 (symmetry)
|
L301,L302,L303,L311,L314 (basis set)
|
L401 (initial MO guess)
|
L502 (SCF)
|
L801,L804 (reordering MOs, LMOs, MOD method, integral transformation)
|
L923 (perturbation selection, SAC/SAC-CI wavefunction, energy, and
        Z-vector)
|   |
|   |
|   |if geometry optimization
|   |
|   L1111 (2-PDM and post-SCF derivatives (including SAC/SAC-CI), CPMOD)
|   |
|   L1002 (CPHF)
```

```
|   |
|   L701,L702,L703,L716 (integral derivatives)
|   |
| *L601 (population and related analysis)*skipped during optimization
|   |
|   |       if  not converged
|   L103--------------------------> to L202 (keeping operators)
|   |       if converged & MacroIter<=N
|   |       --------------------------> to L202 (discarding operators)
|   |                          (N-times)
|   | if converged, or MacroIter=N+1
|   |
L601 (population and related analysis)
|   |
|   L202 (symmetry)
|   |
|   L301,L302,L303,L311,L314 (basis set)
|   |
|   L401 (initial MO guess)
|   |
|   L502 (SCF)
|   |
|   L801,L804 (reordering MOs, LMOs, integral transformation)
|   |
|   L923 (perturbation selection, SAC/SAC-CI wavefunction, energy)
|   |
|   L601 (population and related analysis)
|   |
L9999 (finalizing calculation and output)
```

The details of the SAC/SAC-CI calculation performed by Link923 are described in the rest of this section.

I-D-1. SAC/SAC-CI SD-*R* part

SAC/SAC-CI SD-*R* part consists of main steps and sub-steps summarized in Tables 1 and 2, respectively. The MO repulsion integrals and the Fock matrix information are transferred from Gaussian SCF part. The main routine #SUPER97# drives the whole SAC/SAC-CI program. The SAC(SD) part is common to both SAC/SAC-CI SD-*R* part and SAC-CI general-*R* and high-spin part. Main step involves the steps necessary to calculate SAC and SAC-CI wave functions and one-electron properties calculated therefrom. Sub-step involves interface program, supplemental program, etc. In the following tables

1. Steps are given in the order of job stream.
2. The step below uses the outputs of the steps above as inputs. The computational information is transferred through files.

Table 1. Main steps in the SAC/SAC-CI SD-*R* part of the program

Step	Job	Input	Output

guide	explanations of 1. SAC/SAC-CI program 2. keyword input 3. manual and namelist input 4. input example 5. file numbers and contents		
sacci1	1. control job stream of SAC/ SAC-CI calculation 2. save information about the stream of calculations	1. keywords for calculation	1. stream of calculation
bpres	1. sort MO repulsion integrals from L802 or L804 2. symmetry specification	1. molecular integrals	1. sorted molecular integrals with symmetry
pres	1. generate labels of all linked operators 2. classify linked operators by their symmetry 3. singly excited ci as reference vectors for perturbation selection and as initial vectors 4. selection of linked operators	1. molecular integrals 2. number of active mo 3. molecular symmetry 4. energy threshold for selection	1. labels of linked operators 2. linked operators after selection 3. initial vectors for iterative diagonalization
cimx	1. integrals between linked configurations	1. molecular integrals	1. integrals between linked configurations
cid	1. iterative diagonalization of ci matrix within linked configurations	1. H-matrix 2. S-matrix	1. ci eigenvalues and eigenvectors
das	1. direct diagonalization of ci matrix within linked configurations	1. H-matrix 2. S-matrix	1. ci eigenvalues and eigenvectors
ulintg	1. integrals for unlinked terms in the SAC calculation	1. molecular integrals	1. unlinked integrals for SAC calculation
sac	1. solve SAC non-variational equation (SAC-NV) by iterative procedure	1. H,S-matrix 2. unlinked integral	1. SAC solution
dsac	1. solve SAC non-variational equation (SAC-NV) by iterative procedure	1. H,S-matrix 2. unlinked integral	1. SAC solution
ulints	1. integrals for unlinked terms in singlet SAC-CI calculations	1. molecular integrals	1. SAC-CI unlinked integrals
ulintt	1. integrals for unlinked terms in triplet SAC-CI calculations	1. molecular integrals	1. SAC-CI unlinked integrals
ulintia	1. integrals for unlinked terms in SAC-CI for ionized and electron-attached states	1. molecular integrals	1. SAC-CI unlinked integrals
sciv	1. iterative SAC-CI-V solution --approximate variational—	1. H,S-matrix 2. Unlinked integral	1. SAC-CI-V eigenvalues and eigenvectors
das	1. direct SAC-CI-V solution --approximate variational—	1. H,S-matrix 2. Unlinked integral	1. SAC-CI-V eigenvalues and eigenvectors

scinv	1. iterative SAC-CI-NV solution --non-variational—	1. H,S-matrix 2. Unlinked integral	1. SAC-CI-NV eigenvalues and eigenvectors
dnas	1. direct SAC-CI-NV solution --non-variational--	1. H,S-matrix 2. Unlinked integral	1. SAC-CI-NV eigenvalues and eigenvectors
dens	1. density matrices and natural orbitals for SAC and SAC-CI wave functions 2. transition densities between SAC and SAC-CI wave functions 3. spin density matrices	1. SAC/SAC-CI solutions	1. natural orbitals 2. transition densities 3. spin density matrices
prop	1. one-electron properties 2. transition properties 3. circular dichroism 4. hyperfine splitting constant	1. density 2. natural orbital 3. transition density 4. spin density matrix	1. one-electron properties 2. transition properties 3. circular dichroism 4. hyperfine splitting constant

Note. Steps das and dnas are good for vector processors.

Table 2. Sub-steps in the SAC/SAC-CI program

Step	Job
fock	1. fock matrix for non-canonical orbitals
gsum	1. group sum of linked operators for different geometries. This step is useful for calculating smooth potential surface and analytical energy gradients.
satei	1. intensity of ionization spectrum including shake-up process
iopc	1. transform MyIOp into SAC-CI one (namelist input)
fio	1. file I/O interface
sacutil	1. common subroutines used for integrals and SAC/SAC-CI analytical energy
comcg	1. rewrite the information in common file
time	1. print timing data with messages
input	1. sample input
output	1. output of sample input

GSUM method

To study the properties associated with the potential energy surfaces like

(a) optimized geometry
(b) potential energy surface itself
(c) chemical reaction pathway,
(d) relative energies of the reactant, transition state, intermediate, and product

we have to use the GSUM method when we use the perturbation selection procedure (when the selection threshold is non-zero).

When perturbation selection is done at individual geometries, the resultant potential curve may become discontinuous, so that we must take common set of selected linked and unlinked operators for all the geometries along the potential curve. This method is called GSUM (group sum of operators) method.

For more details, see the account given for the step GSUM and
H. Nakatsuji, J. Ushio, and T. Yonezawa, Can. J. Chem. 63, 1857, (1985).

I-D-2. Job streams of SAC and SAC-CI SD-*R* calculations

SAC
pres--cimx--cid[das]--ulintg--sac[dsac]
SAC-CI SD-*R*: singlet, triplet, doublet (ionized and electron attached)
--cimx--(cid)--ulints(t,ia)--sciv,scinv[das,dnas]--dens--prop

I-D-3. SAC-CI general-*R* and high-spin part

SAC-CI general-*R* and high-spin calculations are performed in the following steps derived partially independently from SAC-CI SD-*R* part (See Section D-4. Job stream). The SAC part is common to both. Namelist input can be done for the following steps.

(1) Steps common to SAC-CI SD-*R* part (mainly for SAC part):
PRES, CIMX, CID, ULINTG, SAC, DSAC,
DAS, DNAS, SCIV, SCINV, SATEI, PROP

(2) Steps for SAC-CI general-*R* and high-spin part:
GHPRES, EGOP, MEGI, GHDENS

SAC-CI general-*R*

Higher-order linked excitation operators up to sextuples are generated by the exponential generation scheme described in the following papers:

H. Nakatsuji, Chem. Phys. Letters, 177, 331 (1991).
H. Nakatsuji, J. Chem. Phys. 83, 713, 5743 (1985).
H. Nakatsuji, J. Chem. Phys. 94, 6716 (1991).

Single excitation operators are included without selection. Doubles are handled as in SD-*R* part. Triple and quadruple-excitation operators are produced as products of single- and double-excitation operators whose coefficients in the SD-CI are larger than given thresholds (CThreEgABAOp= (A1Op=val,A2Op=val), thrma1 for *S*, thrma2 for D). Quintuple- and sextuple-excitation operators are generated as (1*2*2) and (2*2*2) using different thresholds (CThreEgAABAOp= (A1Op=val, A2Op=val), thmma1 for S, thmma2 for D). For B-operators, these thresholds are given by CThreEgAB=(B1Op=val,B2Op=val) and CThreEgAAB=(B1Op=val,B2Op=val). Thus, the accuracy of the exponential generation of the higher R operators in the general-*R* method is expressed by a set of the thresholds (thrma1, thrma2, thmma1, thmma2). These parameters may be different for different ISYM and KSTATE, thrma1(ISYM,KSTATE), etc. The perturbation selection is also applied to the linked operators up to quadruples using the singles and doubles whose coefficients are larger than a given threshold (EThreEgR or eseleg). For quintuple and sextuple excitation operators, perturbation selection is not done.

It is also possible to generate all the higher-operators and then to perform perturbation selection. This procedure is time-consuming and is recommended only for small systems. In the SAC-CI general-*R* and high-spin analytical energy gradients calculations, this procedure should be used.

SAC-CI high-spin

The term "high-spin" is used for quartet to septet spin states in this program. SAC-CI SD-*R* for singlet, doublet and triplet are done, separately, though it is possible to handle singlet to septet spin states by the SAC-CI high-spin part. SAC-CI general-*R* calculation is possible not only for singlet to triplet, but also for high-spin states.

H. Nakatsuji and M. Ehara, J. Chem. Phys. 98, 7179 (1993).

Table 3. Main steps in the SAC-CI general-*R* and high-spin part

step	job	input	output
ghpres	1 generation of lower-order linked excitation operators	1 molecular integrals	1 lower-order linked excitation operators

	2 selection of lower-order operators		after selection
egop	1 generation of higher-order linked excitation operators 2 perturbation selection of higher-order operators	1 molecular integrals	1 higher-order linked excitation operators after selection

Table. Definition of the lower-order and higher-order excitation operators

kstate	Spin multiplicity	lower-order operators generated in #GHPRES#	higher-order operators generated in #EGOP#
1	singlet	singles and doubles	triples to 6-ples
2	triplet	singles and doubles	triples to 6-ples
3	doublet(ionized)	singles and doubles	triples to 6-ples
4	doublet(anionized)	singles and doubles	triples to 6-ples
5	quartet(ionized)	doubles and triples	quadruples to 7-ples
7	quintet	doubles and triples	quadruples to 7-ples
8	sextet(ionized)	triples and quadruples	5-ples to 6-ples
10	septet	triples and quadruples	5-ples to 6-ples

megi	1 construction of integrals for linked and unlinked terms of SAC/SAC-CI	1 molecular integrals	1 linked and unlinked integrals
ghdens	1 density matrix and natural orbitals for SAC and SAC-CI wave functions 2 transition density between SAC and SAC-CI or between SAC-CI states 3 spin density matrix	1 SAC and SAC-CI wave function	1 natural orbitals 2 transition density 3 spin density matrix

** Note **

Some useful functions of SAC-CI SD-*R* part are not available for SAC-CI general-*R* and high-spin part, for example, separation of two electron integrals for small memory and GSUM.

I-D-4. Job streams of SAC-CI general-*R* and high-spin calculations

SAC (this step is necessary)

pres--cimx--cid--ulintg--sac

SAC-CI high-spin: quartet, quintet, sextet, septet

--ghpres--megi--das--ghpres--megi(linked)--megi(unlinked)-
(reference-CI)
--sciv,scinv--ghdens--prop

SAC-CI general-*R*

Type 1: Using exponential generation algorithm for generating higher-operators

singlet state

--ghpres--megi--das--ghpres--megi--sciv-
(reference-CI) (SDCI for determining singlet A-operators)
--egop--megi(linked)--megi(unlinked)--sciv,scinv--ghdens--prop

triplet state

--ghpres--megi--das--ghpres--megi--sciv-
(reference-CI) (SDCI for determining triplet B-operators)

--egop--megi(linked)--megi(unlinked)--sciv,scinv--ghdens--prop

doublet to septet states
Job stream is the same as for triplet state.

Type 2: Generating all the higher-operators (recommended only for small system and energy gradient calculations)
doublet state
--ghpres--megi--das--ghpres--megi--sciv-
(reference-CI) (SDCI for determining doublet B-operators)
--egop--megi(linked)--megi(unlinked)--sciv,scinv--ghdens--prop
In this procedure, SDCI calculation for A-operators is not necessary, when only the doublet states are calculated.

Notes:
(1) A and B- operators are defined as lower-order excitation operators for singlet and other spin symmetries, respectively. They are used for generating higher-order operators in SAC-CI general-*R* method. For SAC-CI high-spin, only B-operator is meaningful and is used for the linked terms.

(2) Reference-CI is performed for generating A- and B- operators. Main configurations of target states should be included in the space of reference-CI. Otherwise, important configurations may be discarded in perturbation selection. Therefore, we recommend SD-reference-CI calculation for SAC-CI general-*R*, even if it is with small active space. See 'RefCIWindow' and the namelist input of &GHPRES.

(3) Higher-order excitation operators are generated in step #EGOP# using exponential generation scheme. Definition of the operators is referred to original article;
H. Nakatsuji, J. Chem. Phys. 94, 6716 (1991).
Higher-order excitation operators are produced as products of lower-order operators, namely, A- and B- operators;
R=B*A, B*A*A, B*A*A*A, ...
Important A and B- operators are selected by preliminary SD-CI calculations. In the present version, A and B- operators of all the space symmetries are used for generating triples and quadruples (R=A*B) and A-operators of all the space symmetries are used for quintuples and sextuples (R=A*A*B).

(4) For calculating the analytical energy gradients of SAC-CI general-*R* and high-spin, one should use Type 2 procedure; namely to generate all the higher-order operators and further to perform perturbation selection.
(See 'FullRGeneration' and &GHPRES ntgenh)

I-D-5. SAC/SAC-CI analytical energy gradient part

(i) Availability and restrictions

SAC/SAC-CI energy gradient is calculated for single specified state even after the energies of many states are calculated.

Analytical energy gradients for SAC/SAC-CI ground and excited states are available for
singlet states,
triplet states,
doublet ionized states,

doublet electron attached (anionized) states,
quartet (ionized) states,
quintet states,
sextet (ionized) states, and
septet states.

For multi-electron excited states like shake-up states, the SAC-CI general-*R* energy gradient calculation is recommended. Calculation of the SAC-CI general-*R* gradients are available for

singlet states (up to quadruple excitations)
triplet states (up to triples)
doublet ionized states (up to quadruples)
electron attached (anionized) states (up to quadruples)
quartet (ionized) states (up to quadruples)
quintet states (up to quadruples).
sextet states (up to quadruples).
septet states (up to quadruples).

For restarting optimization, information of the previous calculation like geometry can be read from check point file.

Non-default unlinked terms (for example, <S(1)|H|S(1)S(2)> and <S(2)|H|S(1)S(2)> integrals for SAC) are not available in the gradient part. Calculation with script-S part is also not available.

Closed-shell Hartree-Fock MOs are adopted for the gradient calculations. To optimize open-shell ground states by the analytical SAC-CI gradients, start with the closed-shell RHF to get reference orbitals for SAC expansion.

Localized molecular orbitals (LMOs) are available. MO derivatives are evaluated by using minimum orbital-deformation (MOD) method explained below in order to avoid singularity in the analytical energy gradient calculations.

Some specificatons for the SAC-CI general-*R* and high-spin gradient calculations:

(1) SAC-CI general-*R* and high-spin gradient calculations are performed by using the routines, some common to but some different from those of the SAC-CI SD-*R* gradient part, in L923 and L1111. In this version, some restrictions exist in the SAC-CI general-*R* gradient part, which are briefly summarized in the following section.
(2) Section D-3 should also be referred to. Job stream is given in D-6.
(3) In the SAC-CI general-*R* and/or high-spin gradient parts, Subroutine ZVItGH (in Step ZVECIT) is called in L923, and Subroutine GenEdm is called in L1111, in which IOp(11/28=-14) are specified by default.
(4) All the higher-order R-operators are generated before perturbation selection in step #EGOP#. See also section D-4. The calculation of higher-order unlinked terms may be skipped. These are automatically set by default, 'FullRGeneration' and 'SkipSmallCI' (in Keyword) or NTGENH=1 and ISKIPH=1 (in Namelist input) Exponential generation algorithm is not available in this step.
(5) During geometry optimization, S- and R-operators selected at the initial geometry are used. (See Sec.(ii), below.)
(6) Geometry optimization using GSUM method is not available in this version.
(7) Analytical energy gradients of sextet and septet states are limited to quadruple excitations.

(ii) Geometry optimization using perturbation selection of operators.

a. Unitary Transformation Freedom within Occupied and Unoccupied MOs versus Perturbation Selection

Perturbation selection of double (and higher) excitation operators used in SAC/SAC-CI method is useful to reduce computational labor, but breaks the invariance of their total energies with respect to the unitary transformations within the occupied and unoccupied subspaces of Hartree-Fock orbitals. For example, the calculated energy is slightly dependent on whether the MOs are canonical or localized, if perturbation selection is done.

Hartree-Fock that defines MO's has a freedom for the unitary transformation within occupied and unoccupied MO's. Hence, two sets of MO's obtained at two near geometries do not necessarily close to each other: the Hartree-Fock MO's may change drastically even though its energy changes very smoothly. Then, we have to introduce a criterion to diminish 'absurd' change of MO's at neighborhood geometry in order to make perturbation selection procedure to be a stable continuous procedure against the geometrical change made in the optimization process. This is the spirit of the minimum orbital-deformation (MOD) procedure introduced in this section. For this purpose, we have to calculate the derivatives of the MO's with respect to the geometrical change. More details are given in I-B, c-15 and c-16.

Derivatives of the conventional MOs with respect to the coordinate can be in many cases extremely large, irrespective of canonical or localized, because MO's have a freedom of unitary transformation within occupied and unoccupied manifolds, and they are not necessarily smooth functions of external parameters like total energy, dipole moment and other observable quantities. In extreme cases, the shapes of the MOs change discontinuously and their derivatives may be even infinity! For example, canonical MOs are defined as diagonalizing the Fock matrix, which is not enough for specifying a particular linear combination of degenerate orbitals. If the degeneracy is relaxed by a perturbation, these MOs are determined in perturbation-dependent manner. Therefore, in the unperturbed limit, these degenerate MOs can be different for different perturbations.

Roughly speaking, the derivatives of the MOs can be expressed in terms of the unperturbed MOs. The perturbation-induced orbital mixing causes the deformation of orbitals, which further causes "unphysical mixing" of the operators (configurations) lying in the selected and discarded manifolds.

This unphysical mixing between selected and discarded configurations of the same excitation level is attributed, as stated above, to occupied-occupied and unoccupied-unoccupied perturbation-induced orbital mixing and if this coupling is unphysically large, the perturbation selection procedure becomes unphysical. Then, it is difficult to use one constant set of selected operator subspace for all the coordinates along the geometry optimization process.

Taking group sum of excitation operators selected along a given reaction pathway, which we call GSUM method, is a simple and useful technique to overcome the above problem in calculating the potential energy curves. In this version, however, the GSUM method is not automatically done in the geometry optimization method, because it is difficult in general to say where is the unknown optimized geometry, without using some physical or chemical considerations. We then use the initially selected operators throughout the geometry optimization processes. After optimization, we again do perturbation selection and repeat optimization using freshly selected operators. This Iteration can be repeated up to three times (once in default). (See "MacroIter" for details.)

b. Minimum orbital-deformation (MOD) method

An alternative method to solve the above-mentioned problem of perturbation selection in

geometry optimization is to eliminate unphysical mixing between selected and discarded operator manifolds. This is accomplished by eliminating perturbation-induced orbital mixing within occupied and unoccupied subspaces, which we call orbital-deformation, since such mixing leads to a change in orbital character.

Provided an initial geometry guess has already been given, we can formulate a method of minimizing orbital-deformation (MOD) in the course of the geometry optimization process by truncating the Taylor expansion of MO coefficients in the neighborhood of a constant reference nuclear configuration. This MOD procedure is described in detail in D-8. This method is formally equivalent to the so called orbital quasidiabatization method.

The SAC/SAC-CI geometry optimization using the energy gradient calculated from the orbitals defined by the minimum orbital-deformation (MOD) method outlined here is available, and actually this method is a default procedure.

c. Default procedure for geometry optimization using perturbation selection within one MacroIteration

```
    Initial geometry written in molecular specification (L101,L103).
    | |
    C L    If LMO is used, calculation proceeds pathway L, C otherwise.
    | |
    SCF (L502).
    | |
    Assign MOs to those for the previous geometry (L801)
    | |
    | Localize MOs (L801).
    | |
    Integral transformation (L804).
    | |
    The linked and unlinked operator subspaces are selected
    by perturbation selection and related method for the
    initial-guess geometry (L923).
    | |
  * The SAC/SAC-CI wave functions are calculated within the
    selected subspace (L923).
    | |
    Gradients are computed (L1111,L1002,L701,L702,L703,L716).
    | |
    Molecular geometry is updated (L103).------------------Exit.
    | |                                                if converged
    | |if not converged
    | |
    SCF (L502).
    | |
    Assign MOs to those of the previous geometry (L801).
    Transform MOs with the MOD method from the reference MOs
    (L801).
    | |
    Integral transformation (L804).
    | |
    Go to * and continue.
```

MacroIteration is explained in D-7 below.

d. Input guide for geometry optimization and remarks

Opt keyword invokes the standard stream of the SAC/SAC-CI geometry optimization shown above.

We recommend to use the MOD method explained above, so that this is default procedure, but if it is necessary to keep CMOs during optimization or potential energy surface calculations (by GSUM), putting CPHF=Canonical outside of SAC-CI keyword is useful. Note that this can cause divergence of gradients when (accidentally) degenerate orbitals happen to exist.

Calculated optimized geometry may be different when different initial guess is used, due to the initial geometry-dependence of the employed operator subspace. The initial geometry guess should be chosen carefully because the perturbation selection is effective only in its neighborhood. Preliminary optimizations at lower levels of theory might be helpful to get good initial-guess geometry.

To reduce the above-mentioned dependence, you can do MacroIteration (up to three times), which is explained in D-7.

(iii) Links invoked for the SAC/SAC-CI gradient calculations

The list of Links invoked to calculate the gradient is shown above (see also I-D). We briefly explain the functions of the Links modified for this method. To describe every details of the Links are out of the scope of this guide and we concentrate ourselves to the points distinct from other post-SCF methods. Readers should refer to User's Reference, Programmer's Reference and the comments in each Links for the structure of the Gaussian suite of programs.

For the SAC/SAC-CI Z-vectors and effective (or relaxed) density matrices, the essence of this theory, readers should also refer to the original papers given in I-B.

Link801

Initializes 2e integral transformation.

Differences from other Post-SCF Methods
(a) Reordering MOs
In doing the GSUM method using CMOs (specified by CPHF=Canonical), the molecular orbitals of different geometries must be corresponded to each other in nature and reordered, if necessary, to have a common sequence of MO's for a series of geometries. For this purpose, reordering MOs is done at the beginning of L801. The SCF results are re-stored to RWF and CHK for the GSUM and geometry optimization steps. If necessary, the sequence of MO's and MO energies are re-ordered, comparing with the last (previous) result.
1. Read the newest SCF results (eigenvectors, eigenvalues, symmetry assignments, etc.) from RWF.
2. Read the last (previous) SCF results from CHK (#20740).
3. Comparing the similarities of eigenvectors between the newest and the last (previous) ones, the sequence of the newest results is re-ordered to be the same as the last ones.
4. Print out summary (IOP(33)=1).
5. Store the newest SCF results in CHK(#20740) and RWF(#740). When #20740 file is empty,

the third step is skipped. This procedure cannot be skipped if CPHF=Canonical is specified.

(b) Localizing MOs
If LMOs are requested and it is the first execution, alpha spin-orbitals are transformed by standard localization procedures, for example, Boys or population (Pipek-Mezey: default) method.

(c) MOD transformation
If MOD method is requested and it is second or later execution (for example, during optimization), MOs are transformed to minimize orbital-deformation as described in D-8 using reference MOs employed for the previous execution.

Link923

Calculates SAC/SAC-CI wavefunction, and then (Step ZVECIT) solves Z-vector equation allowing for non-variational nature of the SAC coefficients.

For data transfer from Overlay 9 to 11, see III-C.

Lnk1111

Constructs 1-particle and 2-particle effective (or relaxed) density matrices (1- and 2-EDM) of the post-SCF methods in MO basis, and then back-transforms them to AO basis. If frozen core approximation is used, 1-EDM is replaced by its canonical version for core-valence block.

Differences from other Post-SCF Methods
(a) For construction of the Lagrangian, only AO-driven scheme is available for SAC/SAC-CI even in full active space because of the absence of anti-symmetrized integrals, (ij//kl).
(b) SAC/SAC-CI SD-*R* EDMs are constructed by SacGam instead of CIGam and CIGL used by other methods.
(c) SAC-CI general-*R* and high-spin EDMs are constructed by GenEdm.
(d) SAC/SAC-CI energy is not invariant to orbital rotations within occupied and unoccupied subspaces of MOs, when the perturbation selection is carried out and near-zero matrix elements are neglected. Additional tasks are required to allow for this breakdown of the invariance. If MOD method is employed, the simultaneous linear equations derived from differentiating the corresponding conditions (see D-8) are solved. See the MOD method explained above. (See also U.J.E. Rice, R.D. Amos, N.C. Handy, T.J. Lee and H.F. Schaefer III, J. Chem. Phys. 55, 963(1986).) If CPHF=Canonical is specified, all 1-EDM elements (not only core-valence block) are replaced by its canonical version.

Link1002

Solves the CPHF (Z-vector) equation.

Differences from other Post-SCF Methods
(a) Only AO-driven scheme (CPHF=AO) is available for SAC/SAC-CI because of the absence of anti-symmetrized integrals, (ij//kl).

I-D-6. Job streams of SAC/SAC-CI analytical gradient calculations

SAC gradients

Link 923 (pres--cimx--cid--ulintg--sac--zvecit)

SAC-CI SD-*R* gradients
Link 923 (pres--cimx--cid--ulintg--sac
--(cimx)--(cid)--ulint(s,t,ia)--sciv,scinv--zvecit)

SAC-CI general-*R* and high-spin gradients
Link 923 (pres--cimx--cid--ulintg--sac
--ghpres--megi--das
(reference-CI: small-active space)
--ghpres--megi--sciv
(SD-CI: large-active space)
--egop--megi(linked)--megi(unlinked)--sciv,scinv--zvecit)

I-D-7. MacroIteration in Geometry Optimization

To reduce the dependence of the optimized result on the perturbation selection, you can do MacroIteration stated below up to three times (default: once).

1. A set of route cards for geometry optimization is shown in D-I.

2. The flow of the route cards is controlled by "MacroIteration=N" which is given from a route section. MacroIteration=N (N=<3) forces to iterate the optimization step N times. The process are shown below focusing the operator selection.

```
(a) Operator perturbation selection for the initial geometry
  |
(b) Geometry optimization                                  <----
  |                                                              |
  |   with keeping the set of selected operators                 N-times
  |                                                              |
(c) Operator perturbation selection at the opt-geometry ---
  |
(d) Single-point SAC-CI calculation at the final opt-geometry
```

I-D-8. Minimization of orbital-deformation

We explain here the method of minimization of orbital-deformation (MOD) that is important for making the perturbation-selected operator manifold stable during the geometry optimization process. The underlying motivation of the MOD method is described in D-5 (ii) above.

Let molecular orbitals be linear combinations of atomic orbitals as

$$\psi_i = \sum_{\mu} \chi_{\mu} C_{\mu i} . \qquad \text{(D-8:1)}$$

We require vanishing dynamical couplings between any real occupied [unoccupied] MOs T_{ij}^{x} [T_{ab}^{x}] defined by

$$T_{ij}^{x} = U_{ij}^{x} - U_{ji}^{x} = 0. \tag{D-8:2}$$

The matrix U^{x} comprising so-called CPHF coefficients satisfies

$$U^{x} = C^{T} S \frac{dC}{dx}, \quad \text{or equivalently} \quad \frac{dC}{dx} = CU^{x}. \tag{D-8:3}$$

In the complete basis set limit, Eq.(D-8:2) is equivalent to

$$\left\langle \psi_i \middle| \frac{d}{dx} \middle| \psi_j \right\rangle = 0, \tag{D-8:4}$$

which is called diabatic conditions. These equations imply that the shapes of the orbitals are kept against the displacement of x. Solving Eq.(D-8:4) exactly is not straightforward. To obtain their approximate solutions, we assume that x is restricted to within the neighborhood of a given x_0, so that Taylor series with respect to the displacement, x-x_0 converges fast. We introduce "displaced" overlap matrix defined by

$$M^{x_0} = C^{x_0 T} S^{x_0} C, \tag{D-8:5}$$

where the constant matrices C^{x_0} and S^{x_0} are equivalent to C and S for x_0, respectively. C^{x_0} is externally given. Truncating the Taylor expansion of C up to first order of the displacements in the neighborhood of x_0, we obtain approximately

$$M^{x_0} = 1 + (x - x_0) U^{x}. \tag{D-8:6}$$

Inserting Eq.(D-8:6) to Eq.(D-8:2) yields approximately

$$0 = T^{x} = U^{x} - (U^{x})^{T} = (x - x_0)^{-1} (M^{x_0} - (M^{x_0})^{T}). \tag{D-8:7}$$

Hence

$$(M^{x_0} - (M^{x_0})^{T}) = 0. \tag{D-8:8}$$

The subset of MOs ψ_i satisfying Eq.(D-8:8) is obtained by the orthogonal transformations of canonical MOs $\{\tilde{\psi}_i\}$ as

$$\psi_j = \sum_i \tilde{\psi}_i W_{ij}^{x_0}, \tag{D-8:9}$$

where the transformation W^{x0} leading to minimum orbital-deformation (MOD) is given by

$$W^{x_0} = \{(\tilde{M}^{x_0})^{T} \tilde{M}^{x_0}\}^{-(1/2)} (\tilde{M}^{x_0})^{T}, \tag{D-8:10}$$

and

$$\tilde{M}^{x_0} = (C^{x_0})^T S^{x_0} \tilde{C}, \qquad \text{(D-8:11)}$$

where $\tilde{C}$ stands for the orbital coefficient matrix for the canonical MOs.

I-D-9. Use of localized molecular orbitals (LMOs)

Several groups report that LMO provides efficient basis to describe electron correlations. It is also the case with SAC/SAC-CI method and the convergence of correlation energy as a function of energy threshold in perturbation selection using LMO is faster than that using canonical MOs (CMOs). We found that the population localization (J. Pipek and P. G. Mezey, J. Chem. Phys. 90, 4916 (1989)) is more efficient than the Boys localization.

In Gaussian system of programs, only the active MOs are localized in Link 801 before integral transformation. Boys and population localizations are available. SCF MOs are overwritten with the LMOs.

Once MOs are localized, notion of "orbital energy" vanishes and SAC/SAC-CI calculation must be performed without assuming diagonal Fock matrix (see NONHF option). It should be noted that "HOMO" and "LUMO" seen in output are meaningless if LMOs are used.

Since localization does not conserve irreducible representation symmetry of MOs, the symmetry in Gaussian may not work correctly and should be disabled completely (see NoSymmetry keyword).

For the ground state, calculation with LMOs is efficient even if the symmetry is disabled. For excited states, however, CMOs are more useful than LMOs when we can use symmetry, since with LMO, symmetry usage is very limited.

In LMO representation, equivalent MOs arise even for molecules with linear symmetry. For example, four CH bond MO's of ethylene are equivalent, and therefore may be treated as "degenerate", but in the present version of SAC-CI program, we do not take such symmetry into consideration (See Section D-10, below).

Optional choice of selection scheme, ISEL=2 is not recommended in combination with LMO, since "main configurations" of SECI are not always distinct in LMO basis.

I-D-10. Perturbation selection for degenerate symmetry

For molecules having degenerate (non-linear) symmetries, the SAC/SAC-CI calculations are performed using closest non-degenerate (linear) symmetry of the subgroup. For example, the molecules of T_d and C_{3v} point group are calculated with D_2 and Cs subgroups, respectively, and the corresponding tables are as follows;

T_d	D_2
A_1	A
A_2	A
E	A
T_1	B_1,B_2,B_3
T_2	B_1,B_2,B_3

C_{3v}	C_s
A_1	A’
A_2	A”
E	A’,A”

This correspondence table between non-linear and linear symmetries is printed out at the top of the SAC-CI calculation.

In SAC/SAC-CI calculations, the perturbation selection is performed for efficient calculations. The degeneracy in non-linear symmetry may not be exactly held when the perturbation selection is independently done for each corresponding symmetry. For example, B_1, B_2, and B_3 states should be exactly degenerate for the T_1 and T_2 states of T_d. To ensure the degeneracy of such states, the perturbation selection is performed as follows for the non-linear symmetry.
(1) When a linked operator is selected, all the other operators which generate the same occupation pattern are selected even if they belong to other space symmetry in the linear group.
(2) The spin functions of the *R*-operators are selected to be complete.

It is also necessary to select the common set of unlinked integrals for the degenerate symmetry. For determining the important *R*-operators of unlinked terms R*S, the SDCI calculations are performed for all the degenerate symmetry, even if the final SAC-CI solutions are not calculated. For examples, when the number of solutions are specified as $(A,B_1,B_2,B_3)=(0,3,0,0)$ for Td, the SDCI calculations are done for $(A,B_1,B_2,B_3)=(0,3,3,3)$; namely, from step PRES to ULINT, number of solutions are set to $(A,B_1,B_2,B_3)=(0,3,3,3)$ and at the end of ULINT, they are changed back to $(A,B_1,B_2,B_3)=(0,3,0,0)$.

Number of solutions of this algorithm is determined by referring to the SECI energy. The SDCI calculations are performed only for necessary states. For example, when only Sigma state is calculated for C*v, the number of solutions of SDCI are set to $(A_1,A_2,B_1,B_2)= (1,0,0,0)$, since the information of Delta state (degenerate state for A1 and A2 in C2v) is not necessary. In calculating the E state of Td, $(A,B_1,B_2,B_3)=(2,0,0,0)$ is set for SDCI, when this E state is lowest in A symmetry and $(A,B_1,B_2,B_3)=(1,0,0,0)$ is specified for SAC-CI.

For saving computational time, different energy thresholds are used for selecting operators that include degenerate orbitals in both occupied (i or j) and unoccpied (a or b) MOs. Default is 3.0*EThreS2G and 3.0*EThreR2. The thresholds for selecting S- and R-operators of the unlinked terms are also relaxed; CThreULS2G, CThreULR1, CThreULR2, CThreULS2E(=0.0), CThreDensULR1, and CThreDensULS2 are multiplied by the factor Sqrt(3.0). These factors of the thresholds can be input by EThreDegFac and CThreDegULFac.

This procedure for non-linear symmetry is also important for the analytical energy gradient calculation to obtain the correct force. In the gradient calculation, however, since linked and unlinked operators are selected only in the initial geometry, the SDCI calculations for all the degenerate symmetry mentioned above are not necessary for the second to last geometries; such SDCI calculations are done only in the initial geometry and the final single point calculation.

For the calculations with LMOs, the point group is C1, but some sets of equivalent MOs appear for molecules with even linear symmetries. For example, four equivalent LMOs exist in Td molecules like CH_4. In ethylene (linear symmetry), four CH bond LMO's are equivalent. However, for the calculations with LMOs, the selection for keeping degeneracy is suppressed in this version because of an increase in computational cost.

The correspondence table for the degenerate symmetry onto the linear symmetry used in the SAC-CI program

---

Symmetry lowering of the degenerate symmetry is due to the following correlation tables. Note that for some non-linear symmetries, two ways of lowering are possible.

(1) C_n groups

$C_3 \to C_1$	$C_4 \to C_2$	$C_5 \to C_1$	$C_6 \to C_2$
$A \to A$	$A \to A$	$A \to A$	$A \to A$
$E \to 2A$	$B \to A$	$E_1 \to 2A$	$B \to B$
	$E \to 2B$	$E_2 \to 2A$	$E_1 \to 2B$
			$E_2 \to 2A$

(2) C_{nv} groups

$C_{3v} \to C_s$	$C_{4v} \to C_{2v}$	$C_{5v} \to C_s$	$C_{6v} \to C_{2v}$	$C_{\infty v} \to C_{2v}$
$A_1 \to A'$	$A_1 \to A_1$	$A_1 \to A'$	$A_1 \to A_1$	$\Sigma^+ \to A_1$
$A_2 \to A''$	$A_2 \to A_2$	$A_2 \to A''$	$A_2 \to A_2$	$\Sigma^- \to A_2$
$E \to A'+A''$	$(B_1,B_2) \to (A_1,A_2)$	$E_1 \to 2B$	$(B_1,B_2) \to (B_1,B_2)$	$\Pi \to B_1+B_2$
	$E \to B_1+B_2$	$E_2 \to 2A$	$E_1 \to B_1+B_2$	$\Delta \to A_1+A_2$
			$E_2 \to A_1+A_2$	---

(3) C_{nh} groups

$C_{3h} \to C_s$	$C_{4h} \to C_{2h}$	$C_{5h} \to C_s$	$C_{6h} \to C_{2h}$
$A' \to A'$	$A_g \to A_g$	$A' \to A'$	$A_g \to A_g$
$E' \to 2A'$	$B_g \to A_g$	$E_1' \to 2A'$	$B_g \to B_g$
$A'' \to A''$	$E_g \to 2B_g$	$E_2' \to 2A'$	$E_{1g} \to 2B_g$
$E'' \to 2A''$	$A_u \to A_u$	$A'' \to A''$	$E_{2g} \to 2A_g$
	$B_u \to A_u$	$E_1'' \to 2A''$	$A_u \to A_u$
	$E_u \to 2B_u$	$E_2'' \to 2A''$	$B_u \to B_u$
			$E_{1u} \to 2B_u$
			$E_{2u} \to 2A_u$

(4) D_n groups

$D_3 \to C_2$	$D_4 \to D_2$	$D_5 \to C_2$	$D_6 \to D_2$
$A_1 \to A$	$A_1 \to A$	$A_1 \to A$	$A_1 \to A$
$A_2 \to B$	$A_2 \to B_1$	$A_2 \to B$	$A_2 \to B_1$
$E \to A+B$	$(B_1,B_2) \to (A,B_1)$	$E_1 \to A + B$	$(B_1,B_2) \to (B_2,B_3)$
	$E_1 \to B_2+B_3$	$E_2 \to A + B$	$E_1 \to B_2+B_3$
			$E_2 \to A+B_1$

(5) D_{nd} groups

$D_{2d} \to C_{2v}$	$D_{3d} \to C_{2h}$	$D_{4d} \to C_{2v}$	$D_{5d} \to C_{2h}$	$D_{6d} \to C_{2v}$
$A_1 \to A_1$	$A_{1g} \to A_g$	$A_1 \to A_1$	$A_{1g} \to A_g$	$A_1 \to A_1$
$A_2 \to A_2$	$A_{2g} \to B_g$	$A_2 \to A_2$	$A_{2g} \to B_g$	$A_2 \to A_2$
$B_1 \to A_2$	$E_g \to A_g + B_g$	$B_1 \to A_2$	$E_{1g} \to A_g + B_g$	$B_1 \to A_2$
$B_2 \to A_1$	$A_{1u} \to A_u$	$B_2 \to A_1$	$E_{2g} \to A_g + B_g$	$B_2 \to A_1$

$E \rightarrow B_1 + B_2$	$A_{2u} \rightarrow B_u$	$E_1 \rightarrow B_1 + B_2$	$A_{1u} \rightarrow A_u$	$E_1 \rightarrow B_1 + B_2$
	$E_u \rightarrow A_u + B_u$	$E_2 \rightarrow A_1 + A_2$	$A_{2u} \rightarrow B_u$	$E_2 \rightarrow A_1 + A_2$
		$E_3 \rightarrow B_1 + B_2$	$E_{1u} \rightarrow A_u + B_u$	$E_3 \rightarrow B_1 + B_2$
			$E_{2u} \rightarrow A_u + B_u$	$E_4 \rightarrow A_1 + A_2$
				$E_5 \rightarrow B_1 + B_2$

(6) D_{nh} groups

$D_{3h} \rightarrow C_{2v}$	$D_{4h} \rightarrow D_{2h}$	$D_{5h} \rightarrow C_{2v}$	$D_{6h} \rightarrow D_{2h}$	$D_{\infty h} \rightarrow D_{2h}$
$A_1' \rightarrow A_1$	$A_{1g} \rightarrow A_g$	$A_1' \rightarrow A_1$	$A_{1g} \rightarrow A_g$	$\Sigma_g^+ \rightarrow A_g$
$A_2' \rightarrow B_1$	$A_{2g} \rightarrow B_{1g}$	$A_2' \rightarrow B_1$	$A_{2g} \rightarrow B_{1g}$	$\Sigma_g^- \rightarrow B_{1g}$
$E' \rightarrow A_1 + B_1$	$(B_{1g},B_{2g}) \rightarrow (A_g ,B_{1g})$	$E_1' \rightarrow A_1 + B_1$	$(B_{1g},B_{2g}) \rightarrow (B_{2g},B_{3g})$	$\Pi_g \rightarrow B_{2g} + B_{3g}$
$A_1'' \rightarrow A_2$	$E_g \rightarrow B_{2g} + B_{3g}$	$E_2' \rightarrow A_1 + B1$	$E_{1g} \rightarrow B_{2g} + B_{3g}$	$\Delta_g \rightarrow A_g + B_{1g}$
$A_2'' \rightarrow B_2$	$A_{1u} \rightarrow A_u$	$A_1'' \rightarrow A_2$	$E_{2g} \rightarrow A_g + B_{1g}$	---
$E'' \rightarrow A_2 + B_2$	$A_{2u} \rightarrow B_{1u}$	$A_2'' \rightarrow B_2$	$A_{1u} \rightarrow A_u$	$\Sigma_u^+ \rightarrow B_{1u}$
	$(B_{1u},B_{2u}) \rightarrow (A_u ,B_{1u})$	$E_1'' \rightarrow A_2 + B_2$	$A_{2u} \rightarrow B_{1u}$	$\Sigma_u^- \rightarrow A_u$
	$E_u \rightarrow B_{2u} + B_{3u}$	$E_2'' \rightarrow A_2 + B_2$	$(B_{1u},B_{2u}) \rightarrow (B_{2u},B_{3u})$	$\Pi_u \rightarrow B_{2u} + B_{3u}$
			$E_{1u} \rightarrow B_{2u} + B_{3u}$	$\Delta_u \rightarrow A_u + B_{1u}$
			$E_{2u} \rightarrow A_u + B_{1u}$	---

(7) S_n groups

$S_4 \rightarrow C_2$	$S_6 \rightarrow C_i$	$S_8 \rightarrow C_2$
$A \rightarrow A$	$A_g \rightarrow A_g$	$A \rightarrow A$
$B \rightarrow A$	$E_g \rightarrow 2A_g$	$B \rightarrow A$
$E \rightarrow 2B$	$A_u \rightarrow A_u$	$E_1 \rightarrow 2B$
	$E_u \rightarrow 2A_u$	$E_2 \rightarrow 2A$
		$E_3 \rightarrow 2B$

(8) Polyhedral groups

$T_d \rightarrow D_2$	$O_h \rightarrow D_{ih}$
$A_1 \rightarrow A$	$A_{1g} \rightarrow A_g$
$A_2 \rightarrow A$	$A_{2g} \rightarrow A_g$
$E \rightarrow 2A$	$E_g \rightarrow 2A_g$
$T_1 \rightarrow B_1 + B_2 + B_3$	$T_{1g} \rightarrow B_{1g} + B_{2g} + B_{3g}$
$T_2 \rightarrow B_1 + B_2 + B_3$	$T_{2g} \rightarrow B_{1g} + B_{2g} + B_{3g}$
	$A_{1u} \rightarrow A_u$
	$A_{2u} \rightarrow A_u$
	$E_u \rightarrow 2A_u$
	$T_{1u} \rightarrow B_{1u} + B_{2u} + B_{3u}$

$T_{2u} \rightarrow B_{1gu} + B_{2u} + B_{3u}$

I-D-11. Integral transformation

AO based integrals are transformed to MO ERIs (electron repulsion integrals) with L804. The SAC/SAC-CI method needs full sets (all occupied and virtual orbitals) of MO ERIs that are stored in symmetry-compressed form. MO ERIs are stored in bucket 4 of RWF. The direct and conventional transformation algorisms can be used. The direct algorism recalculates AO integrals when they are required. The conventional algorism uses AO integrals which are already stored on disk. We recommend the direct algorism and this is the default.

Within the direct transformation, the in-core, fully-direct, and semi-direct algorisms are available. In the default, the program will select the best algorism automatically.

In-core (InCore)	: All AO integrals and intermediate data (partially transformed integrals) are stored in core memory.
Fully-direct (FullDirect)	: AO integrals are recalculated and not stored. Partially transformed integrals are stored in core memory.
Semi-direct (SemiDirect)	: AO integrals are recalculate and not stored. Partially transformed integrals are stored in external disk.

Notes:

The in-core and fully-direct methods would be faster than the semi-direct method because sorting of intermediate data is unnecessary. These methods, however, require core memory enough to store N^4 quantities. The semi-direct method requires less core memory but it requires additional disk space (about N^4) for partially transformed integrals.

I-D-12. Memory and disk space usage in SAC/SAC-CI calculations

1. Memory and Electron Repulsion Integrals (ERIs)

To achieve better performance of SAC/SAC-CI, it is recommended to use appropriate memory size of the system. In the SAC/SAC-CI, ERIs are stored 'in core memory' for fast random access in calculating Hamiltonian matrix elements. For large systems, the storage for ERIs usually dominates the computational memory size. Following remark may be necessary.

(1) ERIs that are zero due to symmetry are omitted.
(2) When the space for ERIs is larger than the memory size of your computer, a bucket-type algorithm is adopted, which is effective only for the SD-*R* part. For details, see explanation in #SDPRES#.
(3) The storage of ERIs is approximately $N*(N-1)/4/Nrep$ words, where N=Nact*(Nact-1)/2, Nact is the active space of SAC/SAC-CI and Nrep is the number of irreducible symmetry representation Memory size should be increased using %MEM or -M-, in large calculations, especially when the message 'Recommend to increase core memory' appears.

2. Disk space and RWF

Many intermediate data and Hamiltonian integrals are stored on RWF. The storage of SAC/SAC-CI files is not affected by "MaxDisk", therefore, when the files exceeds the disk space, job terminates. In large-scale calculations where the size of RWF may exceeds the limit, it is recommended to split RWF using %rwf.

3. Maximum number of configuration

For particularly large calculations, the number of the selected configuration may exceed the default value (100000). In this case, 'MaxR2Op' must be enlarged up to the number of configurations.

I-E. Equivalence of EOM-CC and CC-LRT to SAC-CI

The EOM-CC(1989,1993)[1] and the CC-LRT methods(1979,1990)[2] are equivalent to the SAC-CI method(1978). This was obvious theoretically from the beginning, however, this fact has not been properly understood by some investigators. Here, we give some numerical proofs that show the equivalence of EOM-CC and CC-LRT to SAC-CI both in the SD level. We performed the SAC-CI SD-*R* calculations for CH_2 and CH^+ for which the EOM-CCSD[4] and CCSD-LRT[5] calculations were reported.

We also show that the approximation of neglecting the unimportant unlinked terms and the perturbation selection of the linked operators are both accurate and useful. It should be noted that the program system MEG/EX-MEG[6] coded in 1985 can perform both SAC-CI SD-*R* and general-*R* calculations as special cases of more general MEG/EX-MEG calculations [7-10] without introducing any approximations.

The excitation energies of the singlet and triplet excited states of CH_2 and singlet excited states of CH^+ are compared in Tables 1 and 2, respectively. The basis sets and geometries are identical to those used in the EOM-CCSD and CCSD-LRT calculations. The SAC-CI SD-*R* results obtained without any selections are given in the column under Full. From Table 1 we see that the results of the SAC-CI SD-*R* and EOM-CCSD are identical, and from Table 2 those of the SAC-CI SD-*R* and CCSD-LRT are identical: This is a numerical proof of the equivalence of the three methods.

Table 1. Excitation energy (in eV) of singlet and triplet excited states for CH_2 with 6-31G*

	SAC-CI-NV			EOM-CC	Full-CI
State	Full	#1	#2	[4]	
Singlet					
A_1	0.0	.....	.....	0.0	
	5.844	5.871	5.796	5.844	4.517
	9.120	9.109	9.111	9.120	9.053
A_2	6.101	6.105	6.105	6.101	6.093
B_1	1.668	1.669	1.692	1.668	1.679
B_2	9.692	9.660	9.637	9.692	8.254
Triplet					
A_1	8.389	8.376	8.405	8.389	8.327
A_2	5.300	5.305	5.324	5.300	5.315
B_1	-.344	-.344	-.319	-.344	-.310
B_2	8.382	8.370	8.342	8.382	6.904
	9.304	9.299	9.304	9.304	9.150
CPU time (sec)[a]					
SAC-CI	1m17s	29s	25s		

#1: Unlinked terms of R1*S2 and R2*S2 are included and others are neglected. All the thresholds are zero; EThreS2=EThreR2=CThreULS2G=CThreULR1=CThreULR2=0.0

#2: Unlinked terms are same as #1 and further selection is performed with default thresholds; EThreS2=1.d-6, EThreR2=1.d-7, CThreULS2G=5.d-3, CThreULR1=CThreULR2=5.d-2, CThreULS2E=0.0

Table 2. Excitation energy (in eV) of singlet excited states for CH^+ with [5s3p1d/3s1p].

State	SAC-CI-NV			SAC-CI-V		CC-LRT	full-CI
	Full	#1	#2	#1	#2	[5]	
Σ^+	0.000	.....	.....	.....	.....	0.000	0.000
	9.109	9.120	9.076	9.114	9.074	9.109	8.549
	13.580	13.578	13.582	13.574	13.578	13.580	13.525
Π	3.261	3.265	3.271	3.262	3.268	3.261	3.230
	14.454	14.450	14.479	14.444	14.473	14.454	14.127

#1,#2: Same as those of table 1.

A policy of the SAC/SAC-CI program is we calculate only important terms, and we neglect terms if they are certainly negligibly small. By doing so, we can make programs more efficient, so that we can calculate larger and more complex systems, and the physics and chemistry of the calculated results becomes clearer than otherwise. It is by this virtue that we could have been able to apply our SAC-CI method to the porphyrin systems and to the reaction center of photosynthesis of Rhodopseudomonas viridis. For this purpose, we may introduce the following approximations.

(1) Some classes of unimportant unlinked terms are neglected from the beginning.

(2) The perturbation selection of the linked operators and further the selection among the unlinked terms composed of the selected linked terms are performed.

The accuracy of these approximations is also shown in Tables 1 and 2. #1 means that we adopt the approximation (1) given above, and #2 means that the approximation (2) is further done together with the approximation (1). It is seen that both approximations give reliable results within chemical accuracy. The results of SAC-CI-V method are also given for CH^+, and we can see the reliability of this method.

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I-F. Dimension specification

Array size of the SD-*R* part is determined by the parameters in Table 4. Initial guess of these parameters is given in the first step (bpres), and then they are modified automatically step by step. These parameters are stored in the file "ifscsi".

Table 4. Parameters which determine the array sizes.

parameter	variable
#01	Number of primitive gaussians at scf level. #prop#
#02	Number of ao's.

#03	Number of mo's. #eri#
#04	Number of active mo's used in moeri calculation.
#05	SD-CI dimension after perturbation selection (should be larger than #06).
#06	Unit for i/o transfer (should be larger than the dimension #14 at #das#, #dsac# and #dnas#.)
#07	Number of solutions + maximum number of iterations before "refresh" in #cid#, #sciv#, and #scinv#.
#08	SE-CI dimension without symmetry.
#09	SE-CI dimension with symmetry.
#10	DE-CI dimension without symmetry before perturbation selection.
#11	DE-CI dimension with symmetry before perturbation selection.
#12	DE-CI dimension with symmetry after perturbation selection.
#13	= 2, when kblock='kblock' as ordinary is. = 3, when kblock='double', namely when doubly excited configurations are used as main reference configuration in perturbation selection step.
#14	Dimension in direct diagonalization steps, #dsac#, #das#, and #dnas#.
#15	Maximum number of solutions in direct diagonalization steps, #das# and #dnas#.
#16	Array for integral sorting in #isort#.
#17	Number of transformed 2-electron repulsion integrals (only symmetrically non-zero integrals are stored.)
#18	Number of configurations (before selection) taken into perturbation selection subroutine.

The above parameters are converted to the following numbers in each step, and the converted ones are used for dynamical memory allocation.

```
NAT( 2) = #01
NAT( 4) = #02
NAT( 6) = NAT( 4)*NAT( 4)
NAT( 8) = (NAT( 4)+1)*NAT( 4)/2
NAT(10) = NAT( 4)*7
NAT(12) = NAT( 8)+3
NAT(14) = NAT( 4)*NAT( 8)
NAT(16) = #03
NAT(18) = (NAT(16)+1)*NAT(16)/2
NAT(20) = int(NAT(16)/2)
NAT(22) = #4
NAT(24) = NAT(26)*(NAT(26)+1)/2
NAT(26) = NAT(22)*(NAT(22)+1)/2
NAT(28) = NAT(22)*7
NAT(30) = #05 (should be larger than NAT(32))
NAT(32) = #06 (should be larger than NAT(60))
NAT(34) = #07
NAT(36) = NAT(34)*(NAT(34)+1)/2
NAT(38) = NAT(34)+1
NAT(40) = NAT(34)+3
NAT(41) = NAT(34)*2
NAT(42) = #08
NAT(44) = #09
NAT(46) = (NAT(44)+1)*NAT(44)/2
NAT(48) = NAT(44)*7
NAT(50) = #10
```

NAT(52) = #11
NAT(54) = #12 (will be modified in pres-cimx)
NAT(56) = #13
if NAT(56) =2, then NAT(58) = NAT(32)
if NAT(56) =3, then NAT(58) = NAT(52)
NAT(60) = #14
NAT(62) = NAT(60)*(NAT(60)+1)/2
NAT(63) = NAT(60)*2 (numpac)
NAT(64) = NAT(60)*5 (facom)
NAT(65) = NAT(60)+1 (numpac)
NAT(66) = NAT(60)*6 (numpac)
NAT(68) = #15
NAT(70) = #16
NAT(99) = #17

I-G. Input

Input for the SAC/SAC-CI calculations are done with (standard) keywords, detailed keywords, and namelist form. Standard keywords are explained in the User's Reference of Gaussian. Other more detailed Keywords are summarized, together with the standard ones, in this guide. We recommend to use only the standard keywords for most users. The input is simple in the keyword form, but the flexibility increases in namelist input.

(1) Information of Keyword input is saved at #734 in Link 1.
(2) Information at #734 is transformed into MyIOp(#sacci1#) and then into real variables(#iopc#).
(3) Free format namelist input is done when 'Namelist' keyword is selected. This namelist input is very flexible and explained below, but some new features may not be prepared by namelist (only in keywords) by a historical reason. See also (4) below.
(4) For gradient calculations, some important input (e.g., spin-state-specification) can not be done by namelist input.
(5) When input error is found, this program uses the default input data for the step.
(6) Input priority is in the order of Namelist > Keyword, when contradiction occurs.

Input examples are given in Part V of this Guide, together with the corresponding output. Input 631 - 653 are general instructive examples and will give the user a feeling how the SAC/SAC-CI method is used for studying chemistry and physics involving various electronic states. We will explain in Section I-L of this Guide these instructive sample inputs and summarize the physical and chemical implications of the calculated results.

I-H. Keyword input of SAC-CI in Gaussian suite of programs

I-H-1. Keyword input of SAC-CI

SAC-CI

This keyword requests SAC and SAC-CI calculations [1,2]. SAC calculates symmetry-adapted cluster expansion for singlet closed-shell (ground) state [3] and SAC-CI calculates open-shell singlet excited states, triplet ground and excited states, doublet ionized and doublet electron-attached ground and excited states [4], and from quartet to septet [5] ground and excited states. SAC is always necessary for SAC-CI calculations. The SAC wave function is expressed as

$$\left|\Psi^{\mathrm{SAC}}\right\rangle = \exp\left(\sum_{I=1}^{M} \boldsymbol{C_I S_I}\right)\left|\Phi_0\right\rangle,$$

with a closed-shell determinant Φ_0, which is usually Hartree-Fock, and the SAC-CI wave functions are expressed using the SAC wave function as

$$\left|\Psi^{\mathrm{SAC\text{-}CI}}\right\rangle = \sum_{K=0}^{N} \boldsymbol{d_K R_K}\left|\Psi^{SAC}\right\rangle,$$

where S_I for SAC and R_K for SAC-CI are symmetry-adapted excitation operators, $R_0 = 1$, and C_I and d_K are variable coefficients. The SAC-CI SD(single double)-R method is appropriate for ordinary single-electron excitation, ionization, and electron-attachment processes and the SAC-CI general-R method [6], in which the SAC-CI excitation operators $\{R_K\}$ are composed of single to sextuple excitations, is appropriate for multi-electron processes like two-electron excited states and shake-up ionizations [7]. Perturbation selection is done for the linked operators higher than doubles to reduce computational labor. For molecules having degeneracy, the perturbation selection is done so as to keep the degeneracy. When you calculate a property over different geometries (e.g. potential energy curve), you must take a group-sum of the selected operators over the geometries (see GSUM below), since otherwise the property may be calculated discontinuously. Energy gradient method is available for all the states calculated by the SAC and SAC-CI SD-R method [8], general-R method [9] and high-spin multiplet method [10]. Geometry optimization is possible with a keyword OPT. Detailed explanations and usage of the SAC/SAC-CI program in GAUSSIAN are given in the GUIDE in the present SAC-CI homepage [2]. Note that the so-called EOM-CC and CCLRT methods are theoretically equivalent [2,7] to the SAC-CI method published much earlier.

REFERENCE MO, ACTIVE SPACE, AND INTEGRAL TRANSFORMATION:

SAC/SAC-CI usually uses closed-shell restricted Hartree-Fock (RHF) MO as reference orbital, but restricted open-shell Hartree-Fock (ROHF) MO, MC-SCF MO, etc. can also be used as reference MO when such SCF is performed before the SAC/SAC-CI step. But unrestricted Hartree-Fock (UHF) MO is rejected. Localized (L) MO can be used by doing localization just before the integral transformation. The spin multiplicity and molecular charge used in the SCF step are modified when they are specified in the SAC/SAC-CI step. For gradient calculations and geometry optimizations, only closed-shell RHF MOs are adaptable to the SAC/SAC-CI part.

Rydberg bases are important for studying excited states, in particular, Rydberg excited states. Size of active space is important for the quality of SAC-CI calculations: we recommend to use all-valence active space including Rydberg orbitals (default for active space).

Electron repulsion integrals (ERIs) are transformed within the specified active orbital space and stored in the 'in-core memory' for fast random access in calculating integrals. Zero integrals by symmetry are not stored. To achieve good performance of SAC/SAC-CI, we recommend to use appropriate memory size of your computer with **%mem**. For large systems, the storage of ERIs usually dominates the memory and when the space of ERIs exceeds the memory size, the SAC-CI calculations are done with ERIs separately allocated in memory and disc.

Direct requests to use the direct algorithm for the SAC/SAC-CI SD-R calculations. **Direct** is not compatible with **General-R**, **WithoutR2S2**, **FullUnLinked**, **InCoreDiag**, and **InCoreSAC**. The direct SAC-CI code uses different values of internal thresholds, which correspond to the conventional SAC-CI calculations with **NoUnlinkedSelection** keywords. Therefore, the results obtained with the direct SAC-CI code are usually different from the results with the conventional SAC-CI code. The direct SAC-CI code is efficient and therefore, strongly recommended. (G09.B01 and later) [11]

Direct SAC-CI SD-R LevelThree calculation for singlet states of C_{2v} molecule with double-zeta basis.

```
#SAC-CI(Direct, Singlet=(Nstate=(2,1,3,2)))
        /D95 Pop=Full
```

LMO = *item* requests to use localized MO as reference orbital. Pipek-Mezey LMO (**PM** or **Pipek-Mezy**) is recommended. Boys LMO (**Boys**) is also available.

FC (default) is a synonym of **FrozenCore** and implies that inner-shells are excluded from the active space of the SAC/SAC-CI calculations.

FullActive includes all SCF MOs in the active space, and is a synonym of **Full**.

Window = (*M*, [*N*]) is a synonym of **ReadWindow** =(*M*, [*N*]) and means that the SAC/SAC-CI calculation is done within the *M*-th to *N*-th active orbital space (*M* < *N* in the energy order).

For calculations of ESR hfs constants, 1s-core MO should be included in the active space.

CorePrWindow=(*m*, *n*)

activates the calculation of core-excited/core-ionized states and specifies core orbitals from which an electron is excited or ionized in the core-electron processes; *m* and *n* specifies the range of core orbitals. This keyword is used with the **FullActive** or **Window** keyword to include core-orbitals in the active space. (G09.C01 and later)

Direct SAC-CI SD-R calculation of singlet O1s excited states of CO. (See test966)

```
#SAC-CI(Direct, Singlets=(Nstate=(0,0,1,0),
        FullActive,CorePrWindow=(1,1))
        /cc-pVTZ Pop=Full
```

SAC/SAC-CI KEYWORDS:

SAC-CI **SD-R** calculation may be started with the option **SelecCISonly** to examine the states to be calculated, and at the same time, the size of the calculation (number of linked operators) may be checked with the options **LevelOne/LevelTwo/LevelThree**. Then, full SAC/SAC-CI calculations

are performed using the options given below. Afterwards, the accuracy of the results may be checked by using different basis set and higher Level-options. For multi-electron processes, SAC-CI **General-R** method is more accurate than the **SD-R** method.

ACCURACY

SD-R calculates within singles and doubles linked excitation operators (default).

General-R includes up to sextuple linked excitation operators [6,7].

LevelOne/LevelTwo/LevelThree
thresholds of the perturbation selection of the linked double-excitation operators for SAC/SAC-CI are in levels one, two, and three in increasing accuracy. LevelThree is default. (In LevelOne, EThreS2=1*10-5, EThreR2=1*10-6, in LevelTwo, EThreS2=5*10-6, EThreR2=5*10-7, and in LevelThree, EThreS2=1*10-6, EThreR2=1*10-7)

NoLinkedSelection suppresses perturbation selection for linked operators.

WithoutDegeneracy for degenerate molecules, the perturbation selection in the SD-R calculation is done so as to keep the degeneracy (default), but with this option this special care is made off, for reducing computational time (non-default).

WithoutR2S2 ignores R2S2-type unlinked integrals in SAC-CI calculations. This is effective for reducing computational time of SAC-CI SD-R calculations, though the results are somewhat affected.

NoUnLinkedSelection
suppresses the selection for unlinked operators adopted currently.

FullUnlinked forces to include all types of unlinked terms. All the linked and unlinked terms are included without selection and the SAC-CI is forced to be solved with in-core algorithm.

EgOp requests to generate higher-order (more-than-triple) linked operators in general-R by the exponential generation algorithm (default for single point energy calculation). The highest R is specified by **MaxR (**≤ 6). Then, perturbation selection is done with the thresholds that are the same as those for EThreS2 in LevelOne/LevelTwo/LevelThree.

FullRGeneration requests to generate all higher-order linked operators in general-R with **MaxR** ≤ 4 and then to perform perturbation selection as above. (**EgOp** is usually default in general-R, but this is default for gradient calculations and geometry optimizations.)

SPIN STATE

Singlet = *spin-state-specific sub-keywords*
specifies **singlet** states calculations.

You can also calculate the following spin states.

CationDoublet (a synonym of **Doublet)**

AnionDoublet
Triplet
Quartet
Quintet
Sextet
Septet

For doublet states, see also **AddElectron** and **SubEelectron** options below.

SPIN-STATE-SPECIFIC SUB-KEYWORDS

NState = (*N1*,..,*N8*) sets the number of states *N1*,..,*N8* to be calculated by the SAC-CI method for each irreducible representation 1,..,8 of the point group of the molecule. **NState** = *N* means **NState** = (*N*,*N*,…).

SAC state is always calculated and not included in *N*.

Nk most stable states of k-symmetry are selected from the SECI result in SD-R SAC-CI and from the SDCI result in general-R SAC-CI.

Number of irreducible representation is eight for D_{2h}, which is maximum in abelian group. For C_{2v}, four integers can be specified as **NState** = (*N1*,*N2*,*N3*,*N4*).

For degenerate symmetry, the SAC-CI calculation is done in a closest linear symmetry (D_2 for Td, for example) and **NState** option is given for this linear symmetry (**NState**=(1,2,0,0) for calculating one A_1 (or E) and two T states of Td symmetry). The closest linear symmetry used in default for degenerate symmetry is summarized in SAC-CI Guide [2]. See also **WithoutDegeneracy** option.

You may decide the number of solutions referring to the CIS vectors calculated beforehand of SAC-CI (see keyword **SelecCISonly**.)

MaxR = *N* sets the maximum excitation level, *N*, ($\boldsymbol{N} \leq 6$ for **EgOp**, $\boldsymbol{N} \leq 4$ for **FullRGeneration**) of the linked excitation operators in general-R.

Variational solves the SAC-CI equation by diagonalizing symmetrized matrices. (default)

NonVariational solves the SAC-CI equation for non-symmetric matrices. Note that SAC is always solved ‘non-variationally’.

InCoreDiag forces to solve SAC-CI using in-core algorithms.

Iterative = *item* forces to solve SAC and SAC-CI using iterative algorithms. *Item* specifies initial guess: **SInitial** sets CIS solution and **SDInitial** (default) sets CISD solution as initial guess.

Density requests to calculate density matrices, together with Mulliken population, charge, dipole moment and second moment, for the SAC/SAC-CI states calculated. For other properties, see the whole-state keywords, **AllProperties** and **NoProperty** given below.

SpinDensity requests to calculate spin density matrices. Note that this keyword activates

the keyword **FullActive**.

TransitionDensity/NoTransitionDensity

requests (default) / suppresses calculations of transition density and oscillator strength between SAC ground state and SAC-CI singlet excited states. For other spin-symmetries, the transition density is calculated in default between the lowest SAC-CI state and SAC-CI excited states. (See also TransitionFrom).

SAC-CI SD-R LevelThree calculation for singlet, triplet, and ionized states of C_{2v} molecule with double-zeta basis.

```
#SAC-CI(Singlet=(Nstate=(2,1,3,2)),
        Triplet=(Nstate=(2,1,3,2)),
        CationDoublet=(Nstate=(3,0,2,3)))
        /D95 Pop=Full
```

SAC-CI general-R LevelTwo calculation of the ionized states of a molecule in D_2 symmetry with the R-operators up to quadruples within the active space of the second to 14-th MOs.

```
#SAC-CI(Window=(2,14), LevelTwo, General-R,
        CationDoublet=(Nstate=(3,0,1,1), MaxR=4))
        /D95
```

GRADIENT CALCULATION AND GEOMETRY OPTIMIZATION

TargetState = (SpinState=*Spin*, Symmetry=*M*, Root=*N*)

specifies the target state for which the gradient calculation or geometry optimization is done. The following three items must be specified. *Spin* specifies the spin multiplicity of the target state using one of **Singlet**, **CationDoublet**, **AnionDoublet**, **Triplet**, **Quartet**, **Quintet**, **Sextet**, and **Septet**. *M* specifies the irreducible representation number of the point group, which is defined in the SCF step. *N* specifies the solution number in the desired *Spin-Symmetry* state.

To fix these parameters, we recommend to perform single point SAC-CI calculation before doing the geometry optimization.

When the SAC solution is your target, specify as

TargetState = (**SpinState=Singlet**, **Symmetry=1**, **Root=0)**.

In general-*R*, the generation of the higher-order linked operators is automatically forced to be **FullRGeneration** for gradient calculations and geometry optimizations.

MacroIteration = *N* (*N* ≤ 3)

requests to iterate macro optimization step N-times. MacroIteration=1 is default.

An additional single-point SAC-CI calculation is done after optimization using the optimized geometry.

RELATED KEYWORDS

CPHF = Canonical means that derivatives are evaluated by differentiating the canonical MO set.

CPHF = MOD (default)

means that the derivatives are evaluated by differentiating the minimum orbital deformation (MOD) [12,13] condition to avoid singularities in the energy gradient calculations. See **CPHF**.

Force activates gradient calculation.

Opt activates geometry optimization.

Freq does not work in the SAC and SAC-CI calculations.

Geometry optimization for the second triplet B1 excited state of C_{2v} molecule.

```
#SAC-CI=(Triplet=(NState=(0,0,2,0)),
         TargetState=(SpinState=Triplet, Symmetry=3, Root=2))
         /D95* Opt
```

ODD-ELECTRON MOLECULE AND ROHF ORBITAL

When your target is odd-electron molecule and the SCF procedure is carried out with odd number of electrons, an even-electron closed-shell configuration must be constructed for the SAC method, since SAC is for closed-shell in this program. The following two options are available to modify the open-shell SCF configuration into a closed-shell configuration.

AddElectron requests to add one electron to the open-shell SCF configuration. This is a default action when **CationDoublet**, **Quartet**, and **Sextet** are treated.

SubElectron requests to subtract one electron from the open-shell SCF configuration. This is a default action when **AnionDoublet** is treated.

ROHF MOs of neutral radical may be used and the SAC calculation is done for closed-shell anion (cation), and the ground and excited states of the neutral radical is solved by the SAC-CI method with **CationDoublet** (**AnionDoublet**) option.

```
#SAC-CI(AddElectron, CationDoublet=(NState=(2,1,2,3)))
       /D95 ROHF

#SAC-CI(SubElectron, AnionDoublet=(NState=(2,1,2,3)))
       /D95 ROHF
```

ITERATIVE METHOD

InCoreSAC forces to solve SAC using in-core algorithms.

MaxItDiag = *N* sets maximum number of iterations to *N* for diagonalization.

MaxItSAC = *N* sets maximum number of iterations to *N* in solving SAC equation.

DConvDiag = *M* sets the energy convergence criterion to 10^{-M} in the diagonalizations for SAC-CI and CI.

DConvSAC = *M* sets the energy convergence criterion to 10^{-M} in solving SAC equation

DENSITY AND TRANSITION DENSITY

TransitionFrom = (**SpinState=***Spin*, **Symmetry=***M*, **Root**=*N*)

specifies the initial state for calculating transition density matrices. *Spin*, *M* and *N* work in the same manner as the options in **TargetState**. All states of the same spin-space symmetry calculated are used as the final states.

AllProperties requests to calculate all multipole moments up to hexadecapole, all N-th moment up to fourth-moment, all electrostatic properties, and diamagnetic terms (shielding and susceptibility). This option works for all spin-states for which **Density** is specified.

NoProperty suppresses the calculations of any properties.

GSUM (GROUP SUM OF SELECTED OPERATORS)

When molecular properties are studied over different geometries using perturbation selection, we must take a group-sum (GSUM) of the linked and unlinked operators selected at different geometries, since otherwise the properties may be calculated discontinuously.

BeforeGSUM requests to initialize a series of GSUM calculations. This keyword must be used at the first geometry of the GSUM calculations.

CalcGSUM requests to add the operators selected at current geometry to the group-sum (GSUM) set.

AfterGSUM requests to perform SAC/SAC-CI calculations using the GSUM operators collected at all geometries.

In **CalcGSUM**, the SCF orbitals are re-ordered to be the same, in nature, as the former orbital sequence. This re-ordering is carried out automatically in Link 801.

The same symmetry point group must be used in all GSUM calculations.

BGSUM, **CGSUM**, and **AGSUM** are synonyms of the above keywords.

GSUM is available only for SAC/SAC-CI SD-R calculations of singlet, triplet, ionized, and electron-attached states, not for general-R and high-spin states.

In a series of GSUM calculations, the minimum orbital deformation (MOD) condition is satisfied automatically.

For more details, see GUIDE [2].

Potential energy curves of the singlet excited states of a linear homonuclear molecule are calculated by the GSUM options with canonical orbitals using in-core algorithm.

```
%Chk=Mol
#SAC-CI(BeforeGSUM,Singlet=(NState=(1,0,1,0,0,1,1,0),
         InCoreDiag))
        /D95(d) Unit=Bohr CPHF=Canonical
```

```
 Start GSUM at R=4.0 au.

  0 1
Li
Li 1 4.00

--Link1--

%Chk=Mol
#SAC-CI(CalcGSUM,Singlet=(NState=(1,0,1,0,0,1,1,0),InCoreDiag))
       /D95(d) SCAN Unit=Bohr CPHF=Canonical

Calc. GSUM from R=5.0 to R=12.0 au.

 0 1
Li
Li 1 R1

R1 5.0 7 1.0

--Link1--

%Chk=Mol
#SAC-CI(AfterGSUM,Singlet=(NState=(1,0,1,0,0,1,1,0),InCoreDiag))
       /D95(d) SCAN Unit=Bohr CPHF=Canonical

After GSUM back from R=12.0 to R=4.0 au.

 0 1
Li
Li 1 R1

R1 12.0 8 -1.0
```

MEMORY REQUIREMENT

MaxR2Op = *N* sets maximum number of R2 operators after perturbation selection to *N*. The default number is 100000.

MaxEgOp = *N* sets maximum number of operators in general-R method to *N*. The default number is 5000.

OTHERS

SelecCISonly forces to stop the process after CIS and perturbation selection. The CIS vectors and the numbers of the selected linked-excitation operators are printed out. For SAC-CI calculations of ordinary one-electron excited, ionized, and electron attached states, the target states and the corresponding dimensions of the linked excitation operators are examined using this Keyword before doing full SAC-CI calculations.

SACOnly performs only the SAC calculation and does not compute any excited states.

MORE INFORMATION

Instructive sample inputs and the scientific presentations of the calculated results are given in the SAC/SAC-CI Guide attached at the top of Link 923 [2], together with the detailed explanations of the SAC/SAC-CI method and the algorithms currently adopted. The outputs for the sample inputs are given in the directory g09/tests/.

References

(1) H. Nakatsuji, in Computational Chemistry - Reviews of Current Trends, Vol. 2, ed. J. Leszczynski, World Scientific, 1997, pp.62-124.
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(12) K. Toyota, M. Ehara, H. Nakatsuji, Chem. Phys. Lett. 356, 1 (2002).
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I-H-2. Detailed Keyword input of SAC-CI

Following additional Keyword inputs are also available for detailed control of the SAC/SAC-CI program. These keywords are usually unnecessary; the above standard keywords are recommended.

Detailed Keywords for Selections in both SD-*R* and General-*R* SAC-CI

<Special Keywords only for SAC>

EThreS2 = val — sets energy-threshold (EThre) for perturbation selection of S2 operators.

CThreULS2G = val — sets CThre for S2 in SAC unlinked term.

<Keywords for SAC-CI>

CThreULS2E = val — sets CThre for S2 in SAC-CI unlinked term.

CThreULR1 = val — sets CThre for R1 in SAC-CI unlinked term.

CThreULR2 = val — sets CThre for R2 in SAC-CI unlinked term.

CThreDensULS2 = val — sets CThre for S2 in unlinked term of density calculation.

CThreDensULR1 = val — sets CThre for R1 in unlinked term of density calculation.

CThreMainConfig = val	sets coefficient-threshold (CThre) for choosing main reference configurations used in perturbation selection. This is valid only in case of LinkedSelection=2.
RefCIWindow =(M,[N])	small reference SDCI calculation for perturbation selection is done within the M-th to N-th active orbitals (M < N in energy order). This is used when reference CI active space is specified for calculationg two-electron processes with General-*R* method or with RefSDCI option.
RefCISD	use the CISD solutions as the reference states.
EThreDegFac	sets the factor multiplying on EThreS2 and EThreR2 in the perturbation selection of linked operators for degenerate systems
CThreDegULFac	sets the factor multiplying on CThreDensULS2, CThreULR1, CThreULR2, and CThreDensULR1, in the selection of unlinked operators of degenerate system.

Detailed Keywords for Selections in General-*R* SAC-CI

CThreEgABAOp =(subword)	sets CThre for selecting A and B operators of the A*B term in the exponential generation scheme.
subword	
A1Op = val	sets CThre for A1 operator to var.
A2Op = val	sets CThre for A2 operator to var.
CThreEgAABAOp =(sub-description)	sets CThre for selecting A and B operators of the A*A*B term in the exponential generation scheme.
subword	
A1Op = val	sets CThre for A1 operator to var.
A2Op = val	sets CThre for A2 operator to var.
EgAOp = (subword)	specifies types of CI for generating A-operators from which selection of A-operators is done.
subword	
Type = S	requests CIS for generating A-operators.
= SD	requests CISD for generating A-operators.
ActiveSpace = Small	forces to read active MO space from RefCIWindow.
= Large	forces to read active MO space from Window.
Selection	requests to carry out selection of A-operators.
NoSelection	suppresses selection of A-operators.
EgBOp =(subword)	specifies types of CI for generating B-operators.
subword	
Type = S	requests CIS for generating B-operators.
= SD	requests CISD for generating B-operators.
ActiveSpace = Small	forces to read active MO space from RefCIWindow.
= Large	forces to read active MO space from Window.
Selection	requests to carry out selection of B-operators.
NoSelection	suppresses selection of B-operators.

Detailed Keywords for Special Routes

SAConly	suppresses SAC-CI routes.
NonHF	the MOs used are not canonical, so the Fock matrix is calculated using the given MO set.
SmallCI	requests to carry out a small CI before FullRGeneration.
SkipSmallCI	suppresses SmallCI (default).

SPIN MULTIPLICITY

Spin-state-specific Detailed Keywords for both SD-*R* and general-*R* SAC-CI

LinkedSelection = n	=0: activates perturbation selection using reference states. (default) =1: activates perturbation selection using (coefficients)**2. =2: activates perturbation selection using configurations.
EThreR2 = val	specifies energy-threshold (EThre) for R2 in perturbation selection.
PlusULSAC = (terms)	requests to add unlinked terms in SAC specified by terms in addition to S2S2 used in default.
terms = All, S1S1, S1S2, S1S1S1	
PlusULSACCI = (terms)	requests to add unlinked terms in SAC-CI specified by terms in addition to R1S2 and R2S2 is used in default.
terms = All, R1S1, R2S1	

Spin-state-specific Detailed Keyword for General-*R* SAC-CI

EThreEgR = val	specifies energy-threshold in perturbation for higher-order general-*R* operators.
CThreEgAB =(subword) subword	sets CThre for selecting A and B operators of the A*B terms in the exponential generation (Eg) scheme.
B1Op = val	sets CThre for B1 operator to var.
B2Op = val	sets CThre for B2 operator to var.
CThreEgAAB =(subword) subword	sets CThre for selecting A and B operators of the A*A*B terms in the exponential generation (Eg) scheme.
B1Op = val	sets CThre for B1 operator to var.
B2Op = val	sets CThre for B2 operator to var.
CThreEgULR = var	sets coefficient-threshold (CThre) for selection of unlinked-terms in the exponential generation (Eg) scheme to var.

Spin-state-specific Detailed Keywords for Short-cut Routes

CISonly	forces to carry out CIS calculations using L923.
CISDonly	forces to carry out CISD calculations using L923.

Detailed Keywords for Orthogonalization of SAC-CI with SAC

WithHF	requests to include the Hartree-Fock configuration in SAC-CI solutions (default).
WithoutHF	requests to remove the Hartree-Fock configuration in SAC-CI solutions.
ScriptS	requests to include script-S part in SAC-CI solutions.

Detailed Keywords for Iterative Method

ConvLin = M	sets the energy convergence criterion to 10**(-M) in solving the linear equation of SAC.
MaxItLin = N	sets the maximum iteration to N in solving the linear equation of SAC.
Omega = N	sets a parameter for relaxation method in the linear equation of SAC.
CutoffDIIS = var	sets a cut-off parameter for DIIS in SAC.
CutoffDIISZVec = var	sets a cut-off parameter for DIIS in the Z-vector method.

Detailed Keywords for Print Control

#P	#P requests more printing.
PrintOperator	requests to print out all excitation operators.
PrintNaturalOrbital	requests to print out the natural orbitals.
PrintDensityMatrix	requests to print out the density matrix.
PrintMyIOp	requests to print out MyIOp.

Detailed Keywords for Name-List Input and Restart

Namelist	forces to read namelist input.
Restart	requests to re-start from the last link.

I-H-3. Summary of the Keywords and the Default Action

Keyword	Short explanation	Default action
===== STANDARD KEYWORDS =====		

REFERENCE MO FOR SAC/SAC-CI AND INTERGRAL TRANSFORMATION

LMO	Localized MO	Canonical
FullActive	Full Active Space	Gaussian's standard
Window	Active Space	Gaussian's standard
RefCIWindow	reference CI Window	Window

SAC-CI KEYWORDS:

ACCURACY

SD-*R*/General-*R*	*R*-operators	SD-R
LevelOne/LevelTwo/LevelThree		LevelThree
	Accuracy of calculation of perturbation selection of linked operators	
NoLinkedSelection	Suppress selection	LinkedSelection
FullRGeneration	Generates all higher linked operators in general-*R* SAC-CI	EgOp
WithoutR2S2	Exclude R2S2 unlinked term	not activated
NoUnlinkedSelection	Suppress selection	UnLinkedSelection
FullUnlinked	Include all unlinked terms	S2S2 in SAC R1S2 and R2S2 in SAC-CI

SPIN STATE

Singlet	-	Singlet=NState=1
Triplet	-	Triplet=NState=1
CationDoublet	-	CationDoublet=NState=1
AnionDoublet	-	not calculated
Quartet	-	not calculated
Quintet	-	not calculated
Sextet	-	not calculated
Septet	-	not calculated

SPIN-STATE-SPECIFIC SUB-KEYWORDS

NState	Number of solutions	1
Variational/NonVariational		
	Type of SAC-CI equation	Variational
Iterative=(term)/InCoreDiag		
	Type of diagonalization	Iterative=SDInitial
Density	Density	not calculated
SpinDensity	Spin-density	not calculated
TransitionDensity/NoTransitionDensity		
	TransitionDensity	TransitionDensity
MaxR	Maximum order of R in general-*R*	6 for singlet to quintet 4 for sextet to septet

GRADIENT CALCULATION AND GEOMETRY OPTIMIZATION

TargetState=(...)		
SpinState=spin	Spin-state name	obligatory in OPT/Force
Symmetry=M	Symmetry number	obligatory in OPT/Force
Root=N	Solution number	obligatory in OPT/Force
MacroIteration	Iteration number of optimization	1

RELATED KEYWORDS

CPHF	Type of derivatives	MOD
Force	-	Gaussian's standard
Opt	-	Gaussian's standard
CD	-	Gaussian's standard
ODD-ELECTRON MOLECULE AND ROHF ORBITAL		
AddElectron	Add electron in SAC-CI	
SubElectron	Subtract electron in SAC-CI	
ITERATIVE METHOD		
InCoreSAC	Type of SAC	not activated
MaxItDiag=N	Max. iter. of SAC-CI	64
MaxItSAC=N	Max. iter. of SAC	20
DConvDiag=N	Convergence threshold 10**(-N)	4 for single point 5 for gradient
DConvSAC=N	Convergence threshold 10**(-N)	6 for single point 7 for gradient
DENSITY AND TRANSITIN DENSITY		
TransitionFrom=(...)	Specify initial state	
SpinState=spin	Spin-state name	singlet
Symmetry=M	Symmetry number	1
Root=N	Solution number	0 (SAC state)
AllProperties	All property	not activated
NoProperty	No property	not activated
GSUM(GROUP SUM OF SELECTED OPERATORS		
BeforeGSUM/CalcGSUM/AfterGSUM	Set of GSUM procedure	not activated
MEMORY REQUIREMENT		
MaxR2Op	Buffer of R2 operator	100000
MaxEgOp	Buffer of higher- operator	10000
OTHERS		
SelecCISonly	CIS and selection only	not activated

===== DETAILED KEYWORDS =====

SAC		
EThreS2	Energy thre. of S2	1.d-5/5.d-6/1.d-6 (LevelOne/LevelTwo/LevelThree)
CThreMainConfig	Threshold of main configuration	0.1 (not used for state-selection)
CThreULS2G	Threshold of S2 for unlinked term of SAC	0.005
SAC-CI		
CThreULS2E	Threshold of S2 for unlinked term of SAC-CI	0.0
CThreULR1	Threshold of R1 for unlinked term of SAC-CI	0.05
CThreULR2	Threshold of R2 for unlinked term of SAC-CI	0.05
CThreDensULS2	Threshold of S2 in calculating density	0.005
CThreDensULR1	Threshold of R1 in calculating density	0.1
RefCISD	SDCI for reference-CI	not activated
EThreDegFac	factor of threshold for	3.0

	degenerate system	
CThreDegULFac	factor of threshold for degenerate system	sqrt(3.0)
GENERAL-*R*		
EgOp	Exponential generation for higher R-operator	EgOp
CThreEgABAOp=(...)	Thre. of A-operator for	
A1Op	exponential generation of	0.04
A2Op	A*B and A*A*B	0.04
CThreEgAABAOp=(...)		
A1Op		0.1
A2Op		0.1
EgAOp=(...)	Type of A-operator	
Type=(S,SD)		SD
ActiveSpace=(Small/Large)		Small
Selection/NoSelection		Selection
EgBOp=(...)	Type of B-operator	
Type=(S,SD)		SD
ActiveSpace=(Small/Large)		Small
Selection/NoSelection		Selection
SPECIAL ROUTES		
SAConly	Do only SAC	not activated
NonHF	Use non-canonical MOs	HF
SmallCI/SkipSmallCI	Do small CI when FullRGeneration	SkipSmallCI
SPIN-STATE-SPECIFIC SUB-KEYWORDS FOR SD-*R*		
LinkedSelection	Type of selection	0(state-selection)
EThreR2	Energy thre. of R2	1.d-6/5.d-7/1.d-7 (LevelOne/LevelTwo/LevelThree)
PlusULSAC	Other unlinked terms for SAC	not activated
PlusULSACCI	Other unlinked terms for SAC-CI	not activated
SPIN-STATE-SPECIFIC SUB-KEYWORDS FOR GENERAL-*R*		
EThreEgR	Energy thre. of R	1.d-5/5.d-6/5.d-7 (LevelOne/LevelTwo/LevelThree)
CThreEGAB=(...)	Thre. of B-operator for	
B1Op	exponential generation of	0.04
B2Op	A*B and A*A*B	0.04
CThreEGAAB=(...)		
B1Op		0.1
B2Op		0.1
CThreEgULR	Threshold of unlinked terms for general-*R*	0.1
ORTHOGONALIZATION BETWEEN SAC AND SAC-CI		
WithHF/WithoutHF	Include HF config. in SAC-CI	WithHF
ScriptS	Include script-S part	not activated
ITERATIVE METHOD		
ConvLin=M	Convergence threshold for linear equation;10**(-M)	7
MaxItLin=N	Iter. number of SAC	200

	linear equation	
CutoffDIIS	Cut-off parameter	0.01
CutoffDIISZVec	Cut-off parameter	0.1
PRINT CONTROL		
#P	Extra pringing	not activated
PrintOperator	Print operators	not activated
PrintNaturalOrbitall	Print Natural Orbital	not activated
PrintDensityMatrix	Print Density Matrix	not activated
PrintMyIOp	Print MyIOp control	not activated
NAMELIST INPUT AND RESTART		
Namelist	Use fortran-namelist	not activated
Restart	Restart from top of SAC/SAC-CI	not activated

I-I. Density and transition density calculations

For evaluating one-electron properties and transition properties, the SAC/SAC-CI density and transition density matrices are calculated. Details are given in I-B. ref. d)(1). Density matrix can also be calculated effective density matrix (EDM) using analytical gradients. In the present program, these matrices are calculated using SAC-CI left and right vectors.

Method for calculating these matrices is briefly summarized in the following table. For singlet state, SAC-CI includes Hartree-Fock configuration by default, and the calculation of transition density between SAC-CI states is also possible as well as between SAC and SAC-CI states.

Table. Default of calculating density and transition density matrices.

Singlet state	
Density (WITHHF)	<L|O|R>
Transition density	<SAC|O|R(SAC-CI)>
Transition density among SAC-CI states (see Keyword "TransitionFrom")	<Lg|O|Re><Le|O|Rg>
Other spin multiplicity	
Density	<L|O|R>
Transition density	<Lg|O|Re><Le|O|Rg>

* <L|O|R>=<L1|O|R1>+<L1|O|R2>+<L2|O|R1>+<L2|O|R2>+<L2|O|R1S2>
  <R|O|R>/<R|R>=(<R1|O|R1>+<R1|O|R2>+<R2|O|R1>+<R2|O|R2>+
  <R2|O|R1S2>+<R1S2|O|R1>+<R1S2|O|R1S2>)/<R|R>

* In SAC-CI-V, |R> is identical to |L>: <L|O|R> means terms (<R1S2|O|R1>+<R1S2|O|R1S2>) are not calculated.

* For singlet state, transition density is calculated using 'SCRPTS', since overlap between SAC and SAC-CI should be zero, and the results of 'WITHHF' and 'SCRPTS' are almost the same.

I-J. Restart capability

The program can be restarted in cases (a)the program terminated abnormally and (b)the iterative diagonalization failed to converge. The restarted job starts from the step where the terminated job stopped. Restart of Keyword input means restart from the top of the L923. Restart from each steps

in L923, for example from SCIV, namelist input of &CNTL(RESTART) should be used.

I-K. Some computational remarks

1. Neutral radical

(a) When calculating neutral radical, it is recommended that first, MOs of neutral radical are calculated by the restricted open-shell (RO) HF method and then using these MOs, closed-shell anion or cation is calculated by the SAC method with "NONHF" option. Finally, ground and excited states of neutral radical is calculated by the SAC-CI method as an ionized or electron attached state of this anion or cation.

(b) The ROHF is not adapted to the SAC/SAC-CI energy gradient part. So, in such case, reference MOs of SAC/SAC-CI should be calculated for cation or anion of radical by closed-shell HF method, and do similarly to the above procedure. In this case, "NONHF" option is unnecessary.

2. Dimensions of the SAC/SAC-CI matrices

The SAC/SAC-CI dimensions are functions of the thresholds of the perturbation selection. We recommend to check the dimensions using 'SelecCISonly', before executing through-put calculations.

3. InCoreDirect and Iterative diagonalization

(a) SAC equation (linear equation part)

Both InCoreDirect (DSAC) and Iterative (SAC) method are available.

(b) Diagonalization method

Both InCoreDirect (DAS and DNAS) and Iterative method (CID, SCIV and SCINV) are available for the CI, SAC-CI-V and SAC-CI-NV methods. InCoreDirect method calculates all the states on request, but, for the large calculation, may be difficult because of the limitation of memory storage and cpu time. Iterative method solves the solutions that correspond to the initial-guess vectors which are calculated by SECI or SDCI(step CID) method.

Diagonalization method (InCoreDiag or Iterative) can be specified for each spin state.

(c) Initial guess in the iterative method

Target state may not be obtained if an appropriate initial guess vector is not given. In the SAC-CI SD-*R* method, for essentially singly excited states, SECI prepares initial guess, but for the essentially doubly excited states, you should use 'RefCISD' to prepare initial-guess vectors.

4. Input

For SAC/SAC-CI calculations, Keyword input and namelist input are possible.

The priority of the input is in the order of
Namelist input > Keyword input
when there are some contradictions in the input.

5. Potential energy curve

GSUM method should be used when you use perturbation selection of the excitation operators.

6. Link 801 (reordering MOs)

When GSUM procedure is used, L801 reorders the current Mos according to the previous ones. Therefore, the MOs printed out just after SCF using IOP(5/33)=1 may differ from those used in the SAC-CI and population analysis.

7. SCAN

SCAN is useful for calculating potential energy surface. For getting good correspondence between the present and previous MOs, the geometries are automatically generated with so-called "one stroke" for the SAC/SAC-CI calculations. Note that the step size should be small enough to get correspondence of MOs.

8. Ionized states

In SD-*R* calculation of ionized states, maximum number of solutions is set automatically as that of Koopmans states. Therefore, when calculating many shake-up states, 'RefCISD' should be used.

9. Two-electron process

The SAC-CI general-*R* method is recommended for calculating multiple- electron process. Nonetheless, two-electron process can be described (less accurately) by the SD-*R* method. In such case, main reference double configurations should be identified as well as the main reference single configurations, by doing SDCI beforehand by a direct diagonalization method. H24 unlinked integrals should be included (term3="on" by Keyword or Namelist input). Namely, the input 'Iterative=SDinitial' or "SD-initial" of namelist input in &CNTL is necessary.

10. Active space of general-*R* and high-spin

Reference CI of SAC-CI general-*R* and high-spin is performed by InCoreDirect SDCI, where small active space might become necessary.

11. Target state of general-*R*

In the general-*R*, initial vectors of iterative method and reference operators are determined by SDCI with small active space. Therefore, the target states should be included in the SDCI results.

I-L. Usage of SAC/SAC-CI Program for Typical Scientific Problems
--Instructions using Sample Test Jobs, Input 631–653, 689, 921-925, 965, 966--
Actual input and output lists are given in Part V of this manual.

Input 631 ### H_2O with DZ basis - comparison with full-CI

1. Singlet, triplet, ionized, and electron-attached states of H_2O are calculated by the SAC-CI SD-*R* NV method with DZ [4s2p/2s] basis set. Results are compared with the Full-CI ones, showing the reliability of the SAC-CI method. Reference:H. Nakatsuji, K. Hirao, Y. Mizukami, Chem. Phys. Lett. 179, 555, (1991).
2. Dimension of AO basis is 14. Full active space is used; 5 occupied and 9 unoccupied MOs.
3. Since the basis set does not include the Rydberg functions, the calculated results are not directly compared with the experimental values. See Input 632 below for the calculations including the Rydberg functions.

Table 1. Dimension of linked operators, total energy and excitation energy for the singlet, triplet, ionized, and electron-attached states of H_2O calculated by the SAC-CI and Full-CI (FCI) methods.

State	Orbital Picture[a]	Method	Dim.	Total Energy (Hatree) [b]	Error (mHatree)[c]	E_{ex} (eV)[d]
Singlet states						
XA_1	HF det.	SAC	361	-76.156254	1.61	0.00
		FCI	256474	-76.157866		0.00
$2A_1$	$n \rightarrow 3s$	SAC-CI	361	-75.761035	-1.52	10.75
		FCI	256474	-75.759512		10.84
$3A_1$	$\sigma \rightarrow 3p_y$	SAC-CI	361	-75.454280	3.30	19.10
		FCI	256474	-75.457584		19.06
$1A_2$	$\pi \rightarrow 3p_y$	SAC-CI	192	-75.457584	-0.92	10.73
		FCI	245000	-75.761966		10.80
$1B_1$	$\pi \rightarrow 3s$	SAC-CI	216	-75.840435	-2.14	8.59
		FCI	245776	-75.838288		8.70
$1B_2$	$n \rightarrow 3p_y$	SAC-CI	312	-75.670341	-0.20	13.22
		FCI	254752	-75.670141		13.27
$2B_2$	$\sigma \rightarrow 3s$	SAC-CI	312	-75.568589	2.92	15.99
		FCI	254752	-75.571512		15.96
Triplet states						
$1A_1$	$n \rightarrow 3s$	SAC-CI	417	-75.799083	-1.91	9.72
		FCI	440475	-75.797174		9.82
$2A_1$	$\sigma \rightarrow 3p_y$	SAC-CI	417	-75.568723	-0.80	15.99
		FCI	440475	-75.569523		16.01
$1A_2$	$\pi \rightarrow 3p_y$	SAC-CI	274	-75.780262	-0.34	10.23
		FCI	437640	-75.779926		10.28
$1B_1$	$\pi \rightarrow 3s$	SAC-CI	294	-75.869964	-2.46	7.79
		FCI	437520	-75.867507		7.90
$1B_2$	$n \rightarrow 3p_y$	SAC-CI	410	-75.722134	-0.51	11.81
		FCI	441120	-75.721626		11.87
$2B_2$	$\sigma \rightarrow 3s$	SAC-CI	410	-75.634992	0.85	14.18
		FCI	441120	-75.635841		14.23
Ionized states						
$1A_1$	n	SAC-CI	82	-75.663487	-7.81	13.41
		FCI	232968	-75.655680		13.67
$1B_1$	π	SAC-CI	48	-75.728794	-8.56	11.63

		FCI	223282	-75.720230		11.91
$1B_2$	σ	SAC-CI	66	-75.464478	-4.39	18.82
		FCI	232068	-75.460080		18.99
Electron-attached states						
$1A_1$	3s	SAC-CI	150	-75.959222		5.36
$1B_1$	$3p_x$	SAC-CI	72	-75.321567		22.71
$1B_2$	$3p_y$	SAC-CI	134	-75.870687		7.77

[a] n, σ, and π denote lone-pair($3a_1$), O-H σ bond orbital ($1b_2$), and π orbital on O($1b_1$), respectively.
[b] Total energy in hartree. HF energy is -76.009556 hartree.
[c] Error from FCI energy in m-hartree.
[d] Excitation energies for singlet and triplet states, ionization potentials for ionized states, and vertical electron affinities for electron-attached states.

Input 632 ### H_2O with DZ1P plus Rydberg basis

1. Singlet and triplet excited states of H_2O are calculated with DZ1P plus Rydberg [2s2p] functions. The results compare well with the experimental values.
   References:
   H. Nakatsuji, K. Hirao, Intern. J. Quantum. Chem. 20, 1301, (1981)
   H. Nakatsuji, K. Hirao, Y. Mizukami, Chem. Phys. Lett. 179, 555, (1991).
2. Dimension of AO basis is 34. The active space is full-valence (4 occupied and 28 unoccupied MOs); 1s orbital and its counter part are frozen as core.

Table 2. Excitation energy and oscillator strength for the singlet and triplet excited states for H_2O.

State	SAC-CI			Exptl.	
	Orbital picture	E_{ex}(eV)	Osc.(au)	E_{ex}(eV)	Osc.(au)
Singlet states					
$1B_1$	$\pi \to 3s(OH^*)$, $\pi \to 4s$	7.36	0.0556	7.4,7.49	0.060
$1A_2$	$\pi \to 3p_y$, $\pi \to 4p_y$	9.25	0.0000	9.1	
$2A_1$	$\pi \to 3p_x$, $n \to 3s$	9.71	0.0566	9.67,9.73	0.05
$2B_1$	$\pi \to 3p_z$	9.83	0.0079	10.01,9.996	
$3A_1$	$\pi \to 3p_x$, $n \to 3s$	10.01	0.0449	10.17,10.14	
$3B_1$	$\pi \to 4s$, $\pi \to 3s$	11.24	0.0073		
$1B_2$	$n \to 3p_y$, $n \to 4p_y$	11.63	0.0143		
$2A_2$	$\pi \to 4p_y$, $\pi \to 3p_y$	11.72	0.0000		
$4B_1$	$n \to 3p_x$	12.09	0.0002		
$4A_1$	$n \to 3p_z$	12.13	0.0036		
$5A_1$	$\pi \to 4p_x$	12.91	0.0038		
Triplet states					
$1B_1$	$\pi \to 3s(OH^*)$, $\pi \to 4s$	6.97	-	7.0,7.2	
$1A_2$	$\pi \to 3p_y$, $\pi \to 4p_y$	9.11	-	8.9,9.1,9.2	
$1A_1$	$n \to 3s(OH^*)$, $n \to 4s$	9.39	-	9.3	
$2A_1$	$\pi \to 3p_x$, $\pi \to 4p_x$	9.58	-	9.81,9.80	
$2B_1$	$\pi \to 3p_z$	9.78	-	9.98	
$3B_1$	$\pi \to 4s$, $\pi \to 3s$	10.98	-		
$1B_2$	$n \to 3p_y$, $n \to 4p_y$	11.39	-		
$2A_2$	$\pi \to 4p_y$, $\pi \to 3p_y$	11.49	-		
$3A_1$	$n \to 3p_z$	11.89	-		
$4B_1$	$n \to 3p_x$	12.04	-		
$4A_1$	$\pi \to 4p_x$	12.30	-		

Ionized(Cation doublet) states				
$1B_1$	π	12.19	0.9490	12.61
$1A_1$	n	14.52	0.9519	14.73
$1B_2$	σ	18.88	0.9623	18.55

2. The dipole moments and the second moments of the ground and excited states are summarized in Table 3. The dipole moment shows the direction of the electron-cloud reorganization and the second moment shows the size of the electron cloud giving a criterion whether the state is valence or Rydberg type.

Table 3. Dipole moment (DM) and electronic part of second moment (in au) for H_2O.

State	SAC-CI					
	Orbital picture	DM	Second Moment			
		<r>	$<x^2>$	$<y^2>$	$<z^2>$	$<r^2>$
Singlet states						
XA_1	HF det.	-0.87	5.84	7.41	6.80	20.05
$1B_1$	$\pi \rightarrow$ 3s(OH*), $\pi \rightarrow 4s$	0.67	10.86	14.14	13.77	38.78
$1A_2$	$\pi \rightarrow 3p_y$, $\pi \rightarrow 4p_y$	-0.80	11.77	30.70	13.77	56.24
$2A_1$	$\pi \rightarrow 3p_x$, $n \rightarrow 3s$	-0.19	23.64	15.37	14.46	53.47
$2B_1$	$\pi \rightarrow 3p_z$	-3.44	14.90	17.11	37.02	69.04
$3A_1$	$\pi \rightarrow 3p_x$, $n \rightarrow 3s$	-0.41	26.75	16.48	15.50	58.73
$3B_1$	$\pi \rightarrow 4s$, $\pi \rightarrow 3s$	1.81	19.21	21.67	27.32	68.20
$1B_2$	$n \rightarrow 3p_y$, $n \rightarrow 4p_y$	-0.72	13.28	32.42	13.44	59.13
$2A_2$	$\pi \rightarrow 4p_y$, $\pi \rightarrow 3p_y$	-0.58	14.00	37.46	16.28	67.74
$4B_1$	$n \rightarrow 3p_x$	-0.95	37.26	16.67	15.42	69.35
$4A_1$	$n \rightarrow 3p_z$	-2.79	17.01	17.28	36.90	71.20
$5A_1$	$\pi \rightarrow 4p_x$	-0.71	34.32	17.30	19.09	70.71
Triplet states						
$1B_1$	$\pi \rightarrow$ 3s(OH*), $\pi \rightarrow 4s$	0.51	9.82	13.23	12.63	35.68
$1A_2$	$\pi \rightarrow 3p_y$, $\pi \rightarrow 4p_y$	-0.70	10.98	28.47	13.08	52.54
$1A_1$	$n \rightarrow$ 3s(OH*), $n \rightarrow 4s$	0.52	11.96	13.55	12.04	37.55
$2A_1$	$\pi \rightarrow 3p_x$, $\pi \rightarrow 4p_x$	-0.99	31.45	15.36	14.92	61.73
$2B_1$	$\pi \rightarrow 3p_z$	-3.26	14.53	16.72	36.26	67.52
$3B_1$	$\pi \rightarrow 4s$, $\pi \rightarrow 3s$	1.66	19.66	22.11	26.29	68.06
$1B_2$	$n \rightarrow 3p_y$, $n \rightarrow 4p_y$	-0.46	11.50	27.29	11.90	50.68
$2A_2$	$\pi \rightarrow 4p_y$, $\pi \rightarrow 3p_y$	-0.58	13.97	37.35	16.31	67.62
$3A_1$	$n \rightarrow 3p_z$	-2.95	16.89	16.02	31.35	64.27
$4B_1$	$n \rightarrow 3p_x$	-0.98	36.16	16.40	15.32	67.89
$4A_1$	$\pi \rightarrow 4p_x$	-1.31	38.17	18.05	19.46	75.67
Ionized(Cation doublet) states						
$1B_1$	π	-0.90	3.59	5.77	5.27	14.63
$1A_1$	n	-0.73	4.44	5.68	4.39	14.51
$1B_2$	σ	-1.11	4.51	4.83	5.26	14.61

Input 633 ### Usage of SelecCISOnly

1. Singlet B_{1u} states, $V(\pi,\pi^*)$ and π-3d states of ethylene are calculated by the SAC-CI SD-*R* method with [4s2p1d/2s] basis set plus Rydberg functions [2s2p2d] on the center of molecule.
2. Dimension of AO basis is 68. The active space is full-valence (6 occupied and 60 unoccupied

MOs); 1s orbitals and their counter part are frozen as core.

3. We start SAC-CI SD-*R* calculation with SelecCISOnly to decide states to be calculated, and at the same time, we check the size of calculations (number of linked operators) using options LevelOne/LevelTwo/LevelThree; only the SECI calculations and the perturbation selection of doubles are performed. Numbers of S- and R-operators are printed out. SAC-CI dimensions are given in table 4. It is recommended to use this option especially for large system.

Table 4. SAC-CI dimensions for different levels of calculation.

	LevelOne	LevelTwo	LevelThree
ground	2827	3556	5115
excited B_{1u}	1928	2469	4012

4. Finally, SAC-CI SD-*R* LevelThree calculation is performed. Details of the results are given in Input 634, together with other singlet and triplet excited states and ionized states.

Table 5. SECI and SAC-CI results for the singlet B_{1u} states, $V(\pi,\pi^*)$ and π-3d states of ethylene.

State	Character	SECI	SAC-CI SD-*R*			Exptl.	
		E(eV)	E(eV)	Oscillator strength	Second moment	E(eV)	Oscillator strength
B_{1u}	$V(\pi,\pi^*)$	7.733	8.195	0.364	105.5	ca.8.0	0.34
	$\pi \rightarrow 3d\pi$	9.009	9.246	0.063	222.2	9.33	

Input 634 ### ethylene

1. Singlet, triplet and ionized states of ethylene are calculated by the SAC-CI SD-*R* method with [4s2p1d/2s] basis set plus Rydberg functions [2s2p2d] on the center of molecule. Rydberg states are calculated for n=3.
2. Dimension of AO basis is 68. The active space is full-valence (6 occupied and 60 unoccupied MOs); 1s orbital and their counter part are frozen as core.
3. Numbers of states calculated are set to be larger than those required, since the CIS solutions are used as the initial guess for the iterative diagonalization and the states ordering of CIS is not necessarily correct.
4. "Massage" denotes the dummy atom put on the center of the molecule.
5. "IOP(2/15=-1)" forces to use the symmetry even when the Rydberg functions are placed on the dummy atom.

References:

H. Nakatsuji, J. Chem. Phys. 80, 3703 (1984).
C. C. Ballard, M. Hada, and H. Nakatsuji, Bull. Chem. Soc. Jap. 69, 1901 (1996).
J. Hasegawa, M. Ehara, H. Nakatsuji, Chem. Phys. 230, 23 (1998).

Table 6. Excitation and ionization energies of ethylene.[a]

State	Character	SAC-CI SD-*R*			Exptl.	
		E(eV)	Oscillator strength	Second moment $\langle r^2 \rangle$	E(eV)	Oscillator strength
Ground state		---	---	83.6		
Singlet excited states						
A_g	$\pi \rightarrow 3p\pi$	8.223	0.0	149.0	8.28	
B_{1g}	$\pi \rightarrow 3p\sigma$	7.878	0.0	133.4	7.80	
	$\sigma \rightarrow \pi^*$	8.942	0.0	86.8		

B_{2g}	$\pi \rightarrow 3p\sigma$	7.902	0.0	139.8	7.90	
B_{3g}	$\sigma \rightarrow 3s$	9.836	0.0	121.2	9.51	
A_u	$\pi \rightarrow 3d\pi$	8.890	0.0	193.3		
B_{1u}	$V(\pi, \pi^*)$	8.195	0.364	105.6	ca.8.	0.34
	$\pi \rightarrow 3d\pi$	9.246	0.063	222.2	9.33	
B_{2u}	$\pi \rightarrow 3d\delta$	8.919	0.021	189.3	8.90	
B_{3u}	$\pi \rightarrow 3s$	7.236	0.082	122.3	7.11	
	$\pi \rightarrow 3d\sigma$	8.813	0.005	169.8	8.62	
	$\pi \rightarrow 3d\delta$	8.911	0.050	183.8	8.90	
Triplet states						
A_g	$\pi \rightarrow 3p\pi$	8.060	0.0	141.9	8.15	
B_{1g}	$\pi \rightarrow 3p\sigma$	7.843	0.0	131.9	7.79	
	$\sigma \rightarrow \pi^*$	8.598	0.0	85.7		
B_{2g}	$\pi \rightarrow 3p\sigma$	7.839	0.0	137.2		
B_{3g}	$\sigma \rightarrow 3s$	9.630	0.0	116.8		
A_u	$\pi \rightarrow 3d\pi$	8.884	0.0	192.3		
B_{1u}	$T(\pi, \pi^*)$	4.518	0.0	85.1	4.36	
	$\pi \rightarrow 3d\pi$	9.024	0.0	213.4	8.86	
B_{2u}	$\pi \rightarrow 3d\delta$	8.903	0.0	185.8		
B_{3u}	$\pi \rightarrow 3s$	7.123	0.0	119.0	6.98	
	$\pi \rightarrow 3d\sigma$	8.836	0.0	161.1	8.57	
	$\pi \rightarrow 3d\delta$	8.912	0.0	172.6		
Ionized states						
A_g	$(3a_g)^{-1}$	14.676	0.923[b]	72.3	14.66	
B_{3g}	$(1b_{3g})^{-1}$	13.008	0.932	71.8	12.85	
B_{1u}	$(2b_{1u})^{-1}$	19.500	0.853	72.6	19.23	
B_{2u}	$(1b_{2u})^{-1}$	16.176	0.886	72.8	15.87	
B_{3u}	$(1b_{3u})^{-1}$	10.371	0.951	72.7	10.51	

[a] LevelThree
[b] Monopole intensity for ionized states

Input 635 ### LevelOne, LevelTwo, LevelThree for ethylene

1. Singlet, triplet and ionized states of ethylene are calculated by the SAC-CI SD-*R* method. Details are same as Input 634.
2. Results and cpu time of LevelOne, LevelTwo, and LevelThree calculations are compared.

Table 7. Dimension, excitation/ionization energy, and CPU time in different Levels of approximation for ethylene.

	SAC-CI SD-*R*						Exptl.
	LevelThree		LevelTwo		LevelOne		
State	Dim.	E(eV)	Dim.	E(eV)	Dim.	E(eV)	
Ground state							
	5115	---	3556	---	2827	---	---
Singlet states							
A_g	3599	8.223	2044	8.189	1511	8.155	8.28
B_{1g}	4234	7.878	3327	7.838	2874	7.796	7.80
		8.942		8.874		8.821	
B_{2g}	4420	7.901	3344	7.859	2838	7.821	7.90

B_{3g}	3953	9.836	2545	9.788	1996	9.744	9.51
A_u	2107	8.890	1449	8.853	1168	8.818	
B_{1u}	4012	8.195	2469	8.150	1928	8.108	ca.8.0
		9.246		9.210		9.171	9.33
B_{2u}	1400	8.919	876	8.881	718	8.846	8.92
B_{3u}	3389	7.235	2606	7.193	2174	7.156	7.11
		8.813		8.774		8.738	8.62
		8.911		8.874		8.838	8.90
Triplet states							
A_g	2729	8.060	1636	8.035	1277	8.007	8.15
B_{1g}	5778	7.843	4217	7.807	3550	7.773	7.79
		8.598		8.552		8.511	
B_{2g}	5932	7.839	4257	7.799	3482	7.768	
		9.707		9.664		9.624	
B_{3g}	6127	9.630	3679	9.578	2802	9.555	
A_u	2951	8.884	1725	8.858	1288	8.823	
B_{1u}	3139	4.518	2189	4.524	1873	4.501	4.36
		9.024		8.999		8.964	8.86
B_{2u}	1783	8.903	1050	8.876	818	8.842	
B_{3u}	4519	7.123	3195	7.092	2590	7.066	6.98
		8.836		8.779		8.748	8.57
		8.912		8.859		8.821	
Ionized states							
A_g	330	14.676	322	14.613	314	14.569	14.66
B_{3g}	299	13.008	270	12.932	257	12.882	12.85
B_{1u}	312	19.500	283	19.432	273	19.375	19.23
B_{2u}	297	16.176	277	16.106	265	16.054	15.87
B_{3u}	210	10.371	197	10.333	189	10.297	10.51

CPU time			
SCF(L502)	1.8s	1.8s	1.8s
ERI(L804)	4.6s	4.6s	4.6s
SAC-CI	542s	289s	194s
Energy	428s	223s	146s
Transition Density	114s	66s	48s
Total	9m12s	4m59s	3m24s

[a] Calculation is carried out by Compaq DS20E.

Input 636 ### CO_2 Comparison of LevelOne/Two/Three

1. Singlet, triplet and ionized states of CO_2 (carbon dioxide) are calculated by the SAC-CI SD-*R* method with Huzinaga/Dunning DZ basis set plus polarization [4s2p1d] augmented with Rydberg functions of Dunning/Hay [2s2p] on each atom.
2. Dimension of AO basis is 72. The active space is full-valence (8 occupied and 58 unoccupied MOs); 1s core orbitals and their counter part are frozen as core.
3. The results of LevelThree are compared with experimental values in Table 8. The results and cpu time of LevelOne, LevelTwo, and LevelThree are given in Table 9.
4. Calculation with degenerate symmetry (D*h).

Reference :H. Nakatsuji *Chem. Phys.* 75, 425, (1983).

Table 8. Excitation, ionization, and electron-attachment energies of CO_2.

State	Character	SAC-CI SD-R E(eV)	SAC-CI SD-R Oscillator strength	Exptl. E(eV)	Exptl. Relative intensity
Ground state					
Singlet excited states					
Π_g	$\pi_g \rightarrow \sigma_g$(R)[a]	9.06	--- [b]	8.8	
Σ_u^-	$\pi_g \rightarrow \pi_u$	9.36	--- [b]		
Δ_u	$\pi_g \rightarrow \pi_u$	9.44	--- [b]	9.3- 9.4	
Σ_u^+	$\pi_g \rightarrow \pi_u$(R)	11.31	0.12	11.1-11.2	1.0
Π_u	$\pi_g \rightarrow \sigma_u$(R)	11.42	0.02	11.4-11.6	~0.3
Triplet states					
Σ_u^+	$\pi_g \rightarrow \pi_u$	8.37		8.1	
Π_g	$\pi_g \rightarrow \sigma_g$(R)	8.96		8.3	
Δ_u	$\pi_g \rightarrow \pi_u$	9.94		8.8	
Σ_u^-	$\pi_g \rightarrow \pi_u$	9.36			
Π_u	$\pi_g \rightarrow \sigma_u$(R)	11.33			
Σ_g^+	$\pi_u \rightarrow \pi_u$	11.90			
Δ_g	$\pi_u \rightarrow \pi_u$	12.75		12.4	
Ionized states					
Π_g	π_g	13.56	0.93[c]	13.78	
Π_u	π_u	17.85	0.90	17.56	
Σ_u^+	σ_u^+	18.08	0.91	18.08	
Σ_g^+	σ_g^+	19.41	0.90	19.40	
Electron attached states					
Σ_g^+	σ_g^+	0.13			
Σ_u^+	σ_u^+	0.23			
Π_u	π_u	0.22			
Π_g	π_g	0.51			

[a] (R) denotes Rydberg excited state.
[b] Optically forbidden transition
[c] Monopole intensity

Table 9. Dimension, excitation/ionization energies, and CPU time in different Level of approximation for CO_2.

State	SAC-CI SD-*R* LevelThree Dim.	LevelThree E(eV)	LevelTwo Dim.	LevelTwo E(eV)	LevelOne Dim.	LevelOne E(eV)	Exptl.
Ground state							
	6626		4589		3745		
Singlet excited states							
Π_g	6173	9.057	4562	9.013	3999	8.976	8.8
Σ_u^-	7492	9.356	5974	9.339	5252	9.313	
Δ_u	7492	9.437	5974	9.421	5252	9.397	9.3- 9.4
Σ_u^+	7789	11.307	6111	11.276	5334	11.249	11.1-11.2
Π_u	6581	11.421	4458	11.389	3553	11.360	11.4-11.6
Triplet states							
Σ_u^+	8354	8.373	5304	8.367	4304	8.391	8.1
Π_g	9072	8.964	6548	8.920	5558	8.884	8.3

Δ_u	8020	8.944	5277	8.938	4308	8.971	8.8
Σ_u^-	8020	9.360	5277	9.338	4308	9.397	
Π_u	10753	11.332	7463	11.301	6060	11.272	
Σ_g^+	10403	11.895	6636	11.889	5192	11.875	
Δ_g	10403	12.749	6636	12.742	5192	12.725	12.4
Ionized states							
Π_g	445	13.555	423	13.522	417	13.489	13.78
Π_u	443	17.846	423	17.816	407	17.777	17.56
Σ_u^+	482	18.078	450	18.051	426	18.023	18.08
Σ_g^+	501	19.413	458	19.387	445	19.360	19.40
Electron attached states							
Σ_g^+	1167	0.125	386	0.129	182	0.132	
Σ_u^+	249	0.231	69	0.232	53	0.232	
Π_u	232	0.215	60	0.216	38	0.216	
Π_g	253	0.506	71	0.506	49	0.507	
CPU time[a]							
SCF[b]	2s		2s		2s		
ERI[c]	6s		6s		6s		
SAC-CI	14m29s		7m49s		5m41s		
Total	14m41s		8m 1s		5m53s		

[a] Calculation is carried out by Compaq DS20E.
[b] SCF with L502, converged after 10 cycles.
[c] Integral transformation with L804 and the Direct method.

Input 637 ### Free-Base Porphin

1. Q, B, N, L and M states of free-base porphin are calculated by the SAC-CI SD-*R* method.
2. DZ basis set of Huzinaga [4s2p/2s] is used and the dimension of AO basis is 268.
3. The active space is full-valence (57 occupied and 163 unoccupied MOs): Core MOs (24 occupied and 24 unoccupied) are frozen.
4. Only LevelOne calculation is performed in the sample input; EThreS2=1.d-5 and EThreR2=1.d-6.
5. CPU memory of 700MB is specified with %mem to allocate electron repulsion integrals (ERIs) in core memory. If the core memory is not enough for allocating all the ERIs, according to the available memory, the program will automatically divide the ERIs into appropriate number of units which are sequentially allocated on the core memory.

Table 10. Dimension of Linked operator before and after perturbation selection.

Symmetry	NSol	Dimension of linked operator		
		Before selection	After selection	
			LevelOne	LevelTwo
A_g(SAC)	1	5920901	27395	68387
B_{1u}	4	5916248	62118	101179
B_{2u}	4	5916092	58771	95972
B_{3u}	1	4876572	24353	40305

Table 11. Excitation energy and oscillator strength of Free-Base Porphin. Perturbation selection with "LevelOne"[a] accuracy is used.

State	SAC-CI				Exptl.
	Main configuration	Nature	Eex (eV)	f(Pol) (au)	Excitation (eV)
$1B_{1u}$	$(5b_{3u} \rightarrow 4b_{2g})$-$(2a_u \rightarrow 4b_{1g})$	$\pi \rightarrow \pi^*$	1.77	0.00(x)	1.98(Q_x;very weak)

$1B_{2u}$	$(5b_{3u}\rightarrow 4b_{1g})$-$(2a_u\rightarrow 4b_{2g})$	$\pi\rightarrow\pi^*$	2.25	0.00(y)	2.42(Q_y;very weak)
$2B_{1u}$	$(2a_u\rightarrow 4b_{1g})$+$(5b_{3u}\rightarrow 4b_{2g})$ -$(4b_{3u}\rightarrow 4b_{2g})$	$\pi\rightarrow\pi^*$	3.58	1.18(x)	3.33(B;strong)
$2B_{2u}$	$(2a_u\rightarrow 4b_{2g})$+$(5b_{3u}\rightarrow 4b_{1g})$	$\pi\rightarrow\pi^*$	3.71	1.69(y)	3.65(N;broad)
$3B_{1u}$	$(4b_{3u}\rightarrow 4b_{2g})$	$\pi\rightarrow\pi^*$	4.14	0.78(x)	4.25-4.67(L;weak)
$3B_{2u}$	$(4b_{3u}\rightarrow 4b_{1g})$	$\pi\rightarrow\pi^*$	4.33	0.27(y)	4.25-4.67(L;weak)
$1B_{3u}$	$(7b_{2u}\rightarrow 4b_{1g})$	$n\rightarrow\pi^*$	4.42	0.00(z)	4.25-4.67(L;weak)
$4B_{2u}$	$(3b_{3u}\rightarrow 4b_{1g})$	$\pi\rightarrow\pi^*$	4.85	0.30(y)	5.0-5.5(M;weak)
$4B_{1u}$	$(3b_{3u}\rightarrow 4b_{2g})$	$\pi\rightarrow\pi^*$	4.92	0.41(x)	5.0-5.5(M;weak)

[a]"LevelOne" denotes accuracy of EThreS2=1.d-5 and EThreR2=1.d-6 in the perturbation selection.

6. The $5b_{3u}$, $2a_u$, $4b_{2g}$, and $4b_{1u}$ MOs are Gouterman's four orbitals. Adding $4b_{3u}$ orbital to the four orbitals, five orbitals are defined, of which the excitations in the Q, B, and N bands are described.
7. Note on the oscillator strength and polarization. To compare with the experimental polarization using the conventional notation, the directions x and z should be exchanged.
8. Including polarization functions and Rydberg functions gives small amount of shift in the excitation energy.

References:

H. Nakatsuji, J. Hasegawa, and M. Hada, J. Chem. Phys. 104, 2321, (1996).
Y. Tokita, J. Hasegawa, and H. Nakatsuji, J. Phys. Chem. A102,1843, (1998).

Table 12. Excitation energy, oscillator strength, and CPU time in different Level of approximation for free-base porphin.

State	SAC-CI				Exptl.
	LevelOne		LevelTwo		Excitation energy (eV)
	E_{ex} (eV)	f(Pol) (au)	E_{ex} (eV)	f(Pol) (au)	
$1B_{1u}$	1.77	0.00	1.85	0.00	1.98(Q_x;very weak)
$1B_{2u}$	2.25	0.00	2.30	0.00	2.42(Q_y;very weak)
$2B_{1u}$	3.58	1.18	3.70	1.14	3.33(B;strong)
$2B_{2u}$	3.71	1.69	3.86	1.72	3.65(N;broad)
$3B_{1u}$	4.14	0.78	4.27	0.93	4.25-4.67(L;weak)
$3B_{2u}$	4.33	0.27	4.45	0.30	4.25-4.67(L;weak)
$1B_{3u}$	4.42	0.00	4.59	0.00	4.25-4.67(L;weak)
$4B_{2u}$	4.85	0.30	4.98	0.32	5.0-5.5(M;weak)
$4B_{1u}$	4.92	0.41	5.09	0.37	5.0-5.5(M;weak)
CPU time[a]					
SCF(L502)	5m26s		5m26s		
ERI(L804)	19m23s		19m15s		
SAC-CI	2h23m18s		8h10m42s		
Energy	2h09m15s		7h17m04s		
Transition Density	14m03s		53m38s		
Total	2h48m10s		8h35m26s		

[a] Calculation is carried out by Compaq DS20E.

Input 638 ### Geometry optimization of ground and exited states

1. Geometry optimization is performed for the ground and singlet A" excited states of HCF by the SAC/SAC-CI SD-R method. Initial guess geometry is experimental one.

2. DZ1P[4s2p1d/2s] basis set is used and the dimension of AO basis is 34. Full active space is used; 8 occupied and 26 unoccupied MOs.
3. MacroIter=1 (default) is used: one cycle of optimization with perturbation selection at initial geometry and an additional single-point SAC/SAC-CI calculation.
4. The MOD (minimum-orbital deformation) method with the canonical MOs (CMOs) at the initial geometry is used (default).

Table 13. Optimized structure and energy of the ground and singlet A" excited states of HCF.

Method	R(H-C) (Angstrom)	R(C-F) (Angstrom)	∠HCF (degree)	T_e / T_0 [a] (eV)	Total energy (au)
X A' ground state					
SAC	1.126	1.322	102.1	-	-138.07251
Exptl.	1.138	1.305	104.1	-	-
A A" excited state					
SAC-CI	1.103	1.312	123.4	2.396	-137.98445
Exptl.	1.063	1.308	123.8	2.142	-

[a] Theoretical adiabatic excitation energy is given by T_e and experimental one by T_0.

5. Geometries of the ground and excited states are reasonably well calculated and the vertical and adiabatic excitation energies compare well with experiments.
6. Energy value in parentheses is the optimized value and without parentheses is the single-point SAC-CI energy after optimization.

Input 639 ### Geometry optimization of open-shell molecule

1. Geometry optimization is performed for NH_2, an open-shell molecule; X^2B_1 (ground) and A^2A_1 (excited) states of NH_2 are optimized by the SAC/SAC-CI SD-*R* method.
2. DZ1P[4s2p1d/2s1p] basis set is used and the dimension of AO basis is 25. Full active space is used; 5 occupied and 15 unoccupied MOs.
3. MacroIter=1 is used.
4. The MOD method with the canonical MOs of the closed-shell system (NH_2^-) at the initial geometry is used.
5. Results of D95(d,p) and cc-pVTZ are compared in table 14. Calculation with cc-pVTZ gives better results in both equilibrium structure and adiabatic excitation energy.
6. Energy value in parentheses is the optimized value and without parentheses is the single-point SAC-CI energy after optimization.

Table 14. Optimized structure and energy of the X^2B_1 (ground) and A^2A_1 (excited) states of NH_2.

Method	R(N-H) (Angstrom)	∠HNH (degree)	T_e / T_0 [a] (eV)	Total energy (au)
X^2B_1 ground state				
D95(d,p)	1.029	103.4	-	-55.74029 (-55.74028)
cc-pVTZ	1.022	103.5	-	-55.77618 (-55.77606)
Exptl.	1.024 (1.025)	103.36 (102.9)	-	-
A^2A_1 excited state				
D95(d,p)	0.997	145.1	1.470	-55.68625 (-55.68624)
cc-pVTZ	0.979	143.6	1.377	-55.72558 (-55.72551)

Exptl.	0.976	144	1.271	-

[a] Theoretical adiabatic excitation energy is given by T_e and experimental one by T_0.

Input 640 ### MoS_4^{2-} Transition metal, Degeneracy

1. Singlet excited states of MoS_4^{2-} are calculated by the SAC-CI SD-R method with LanL2DZ basis set.
2. Dimension of AO basis is 54. The active space is full-valence (20 occupied and 34 unoccupied MOs), since ECP is used.
3. Results of LevelOne, LevelTwo, and LevelThree are compared. Only LevelOne calculation is executed in the sample.
4. Calculation with degenerate symmetry (T_d).

Table 15. Dimension, excitation energy, and CPU time in different level of approximation for MoS_4 dianion.

	SAC-CI SD-R						Exptl.[a]
	LevelThree		LevelTwo		LevelOne		
State	Dim.	E(eV)	Dim.	E(eV)	Dim.	E(eV)	
Ground state							
	24010	---	13183	---	9123	---	---
Singlet excited states							
$1T_1$	27700	2.305	19758	2.285	16700	2.258	2.37
$1T_2$	27700	2.715	19758	2.692	16700	2.662	2.65
1E	21826	3.612	15131	3.553	12448	3.506	
$2T_1$	27700	3.584	19758	3.529	16700	3.480	3.22
$2T_2$	27700	3.750	19758	3.692	16700	3.637	ca.3.91
CPU time							
SCF(L502)		1s		1s		1s	
ERI(L804)		4s		4s		4s	
SAC-CI		48m48s		22m16s		14m56s	
Energy		2629s		1199s		804s	
Transition density		299s		137s		92s	
Total		49m48s		22m53s		15m25s	

	LevelTwo (WithoutDegeneracy)		Exptl.[a]
	Dim.	E(eV)	
Ground state			
	10494	---	---
Singlet excited states			
$1T_1$	15063,15274,15107[b]	2.301,2.287,2.306	2.37
$1T_2$	15063,15274,15107	2.739,2.699,2.743	2.65
1E	12941	3.536,3.561	
$2T_1$	15063,15274,15107	3.576,3.554,3.576	3.22
$2T_2$	15063,15274,15107	3.740,3.731,3.739	ca.3.91
CPU time[c]			
SCF(L502)	1s		
ERI(L804)	4s		
SAC-CI	12m8s		
Energy	631s		
Transition density	97s		

Total	12m22s

[a] A. Mueller, E. Diemann, Chem. Phys. Lett. 9 (1971) 369.
[b] T_1 and T_2 states are calculated by B_1, B_2, and B_3 states of D_2.
[c] Timing data is given for the calculation only for the B_1 states.

Input 641 ### s-trans-glyoxal O=CH-CH=O (CMO), Levels1/2/3

1. Singlet, triplet and ionized states of s-trans-glyoxal are calculated by the SAC-CI SD-*R* method with TZ basis of Ahlrichs plus Huzinaga's polarization functions [5s3p3d/3s1p].
2. Dimension of AO basis is 108. The active space is full-valence (11 occupied and 93 unoccupied MOs); 1s orbitals are frozen as core.
3. Results of LevelOne, LevelTwo, and LevelThree are compared. Only LevelTwo calculation is executed in the sample.

Table 16. Dimension and excitation/ionization energy for s-trans-glyoxal.

State	Character	SAC-CI SD-*R* Dim.	E(eV)	Oscillator strength	Exptl. E(eV)	Intensity
Ground state		55363				
Singlet excited states						
A_u	$n^{+[a]} \rightarrow \pi^*$	24551	3.03	---[e]	2.8	
B_g	$n^{-[b]} \rightarrow \pi^*$	28298	4.45	0.0002	4.2	weak
Triplet states						
A_u	$n^+ \rightarrow \pi^*$	30328	2.64		2.38	
Ionized states						
A_g	n^+	2716	10.58	0.94[f]	10.60	
B_u	n^-	2719	12.38	0.91	12.20	
B_g	$\Pi^{-[c]}$	1961	14.17	0.93	14.03	
A_u	$\Pi^{+[d]}$	1959	15.68	0.92	15.50	

[a] n-orbital with same phase combination.
[b] n-orbital with reversed phase combination.
[c] π-orbital with reversed phase combination.
[d] π-orbital with same phase combination.
[e] Optically forbidden transition.
[f] Monopole intensity for ionized states.

Table 17. Dimension, excitation/ionization energy, and CPU time in different Level of approximation for s-trans-glyoxal.

	SAC-CI SD-*R*						Exptl.
	LevelThree		LevelTwo		LevelOne		
State	Dim.	E(eV)	Dim.	E(eV)	Dim.	E(eV)	
Ground state							
	55363	---	24399	---	14667	---	---
Singlet states							
A_u	24551	3.033	14110	2.904	10378	2.778	2.8
B_g	28298	4.452	16177	4.361	11815	4.254	4.2
Triplet states							
A_u	30328	2.645	15629	2.572	11056	2.509	2.38
Ionized states							
A_g	2716	10.582	2343	10.363	2107	10.193	10.60
B_u	2719	12.384	2336	12.195	2129	12.034	12.20
B_g	1961	14.169	1652	14.063	1485	13.957	14.03

A_u	1959	15.683	1668	15.578	1471	15.479	15.50
CPU time[a]							
SCF[b]		32s		32s		32s	
ERI[c]		54s		54s		54s	
SAC-CI		1h19m24s		22m33s		10m54s	
Total		1h20m54s		24m 3s		12m24s	

[a] Calculation is carried out by Compaq DS20E.
[b] SCF with L502, converged after 11 cycles.
[c] Integral transformation with L804 and the Semi-Direct method.

Input 642 ### LMO

1. Pipek-Mezey localized MOs (LMOs) are used for SAC-CI SD-R method.
2. D95 basis: AO dimension is 48. Active space: full-valence (11 occupied and 29 unoccupied MOs) 1s orbitals and their counter part are frozen as core.
3. Electron correlations are effectively calculated using the perturbation selection with LMOs, as seen by comparing with the calculation using the canonical MO.

Table 18. Dimensions and energy (in au) of the ground and A" excited state of acrolein.

	CMO	LMO	full linked term[a]
Ground state			
Dim. #S[b]	17102 (C_s)	5925 (C_1)	51359 (C_1)
E(corr.)	-0.34644	-0.38384	-0.38884
E(total)	-191.04976	-191.08715	-191.09215
Excited state			
Dim. #R[c]	7076 (C_s)	5064 (C_1)	51359 (C_1)
E(total)	-190.90577	-190.94187	-190.94288
Excitation energy (eV)	3.92	3.95	4.06

[a] Unlinked terms were selected with normal thresholds.
[b] #S = Number of S-operators
[c] #R = Number of R-operators

Input 643 ### With FullUnlinked keyword

1. All the linked and unlinked terms within the SAC-CI SD-*R* method are calculated using "FullUnlinked" keyword.
2. The singlet and triplet states of CH_2 are calculated with 6-31G* basis. The dimension of AO basis is 19 and the active space is full-valence (3 occupied and 14 unoccupied MOs).
3. The singlet states of CH^+ are calculated with [5s3p1d/3s1p] basis. The dimension of AO basis is 26 and the active space is full: (3 occupied and 23 unoccupied MOs).
4. The results numerically show that both EOM-CC and CC-LRT methods are equivalent to the SAC-CI method.
5. For detailed explanation, see section I-E.

Table 19. Excitation energy (in eV) of singlet and triplet excited states for CH_2 with 6-31G*.

	SAC-CI-NV			EOM-CC	Full-CI
State	Full	#1	#2		
Singlet					

A_1	0.0	.....	.....	0.0	
	5.844	5.871	5.796	5.844	4.517
	9.120	9.109	9.111	9.120	9.053
A_2	6.101	6.105	6.105	6.101	6.093
B_1	1.668	1.669	1.692	1.668	1.679
B_2	9.692	9.660	9.637	9.692	8.254
Triplet					
A_1	8.389	8.376	8.405	8.389	8.327
A_2	5.300	5.305	5.324	5.300	5.315
B_1	-.344	-.344	-.319	-.344	-.310
B_2	8.382	8.370	8.342	8.382	6.904
	9.304	9.299	9.304	9.304	9.150
CPU time (sec)[a]					
SAC-CI	1m17s	29s	25s		

#1: Unlinked terms of R1*S2 and R2*S2 are included and others are neglected. All the thresholds are zero; EThreS2=EThreR2= CThreULS2G=CThreULR1=CThreULR2=0.0

#2: Unlinked terms are same as #1 and further selection is performed with default thresholds; EThreS2=1.d-6, EThreR2=1.d-7, CThreULS2G=5.d-3, CThreULR1=CThreULR2=5.d-2, CThreULS2E=0.0

[a] InCoreDiag is used.

Table 20. Excitation energy (in eV) of singlet excited states for CH^+ with [5s3p1d/3s1p].

State	SAC-CI-NV			SAC-CI-V		CC-LRT	full-CI
	Full	#1	#2	#1	#2		
Σ^+	0.000	.....	.....	.....	.....	0.000	0.000
	9.109	9.120	9.076	9.114	9.074	9.109	8.549
	13.580	13.578	13.582	13.574	13.578	13.580	13.525
Π	3.261	3.265	3.271	3.262	3.268	3.261	3.230
	14.454	14.450	14.479	14.444	14.473	14.454	14.127

#1,#2: Same as those of table 1.

Input 644 ### Group SUM (GSUM) method for potential curve

1. Potential energy curves of Li_2 are calculated with D95(d) basis by the GSUM method.
2. Dimension of AO basis is 32 and the active space is full (3 occupied and 29 unoccupied MOs).
3. "BeforeGSUM" and "CalcGSUM" perform the selections of *R*-operators, and take group-sum of operators before the SAC-CI. "AfterGSUM" performs the SAC-CI calculation with the group-summed operators.
4. "BeforeGSUM" and "CalcGSUM" are done from R=4 to 12 au doing MO correspondence, and "AfterGSUM" calculates the potential curves of Li_2 in the reverse order from R=12 to 4 au.

Table 21. Potential energy curves of the singlet excited states of Li_2 calculated by the SAC-CI GSUM method.

R (au)	SAC Energy (au)	SAC-CI Energy (au)			
	Σ_g^+	Σ_g^+	Π_g	Σ_u^+	Π_u
4.0	-14.902704	-14.788103	-14.776168	-14.821983	-14.792697
5.0	-14.917041	-14.815632	-14.804758	-14.849824	-14.815775
6.0	-14.912301	-14.823251	-14.815364	-14.855335	-14.818671
7.0	-14.902413	-14.823582	-14.818512	-14.851747	-14.815142
8.0	-14.893341	-14.821492	-14.818983	-14.844966	-14.811672

9.0	-14.886995	-14.817996	-14.818557	-14.837707	-14.810030
10.0	-14.883357	-14.814153	-14.817866	-14.831281	-14.809739
11.0	-14.881443	-14.811250	-14.817132	-14.826187	-14.810046
12.0	-14.880483	-14.809795	-14.816450	-14.822462	-14.810520

Table 22. Spectroscopic constants of the singlet states of Li_2.[a]

State Source	$T_e(T_0)$ (eV)	R_e (A)	D_e	ω_e	$\omega_e\chi_e$	B_e	α_e
$X\Sigma_g^+$							
D95(d)	0.0	2.695	8212	350.0	2.59	0.663	0.006
cc-pVTZ	0.0	2.689	8767	346.3	2.49	0.666	0.007
Exptl.[b]	0.0	2.673	8541	351.4	2.58	0.672	0.007
$A\Sigma_u^+$							
D95(d)	1.674(1.680)	3.149	9086	259.8	1.50	0.486	0.005
cc-pVTZ	1.715(1.721)	3.124	9304	254.6	1.66	0.493	0.006
Exptl.[b]	1.74	3.108	8940 (9469)	255.4	1.58	0.498	0.005
$B\Pi_u$							
D95(d)	2.665(2.671)	3.035	2019	254.0	4.24	0.523	0.010
cc-pVTZ	2.550(2.555)	2.956	3287	270.3	3.11	0.551	0.008
Exptl.[b]	2.53	2.935	3102	270.1	2.67	0.558	0.008
$1\Pi_g$							
D95(d)	2.654(2.670)	4.152	1181	84.6	1.87	0.279	0.011
cc-pVTZ	2.697(2.713)	4.052	1381	95.6	1.78	0.293	0.009
$2\Sigma_g^+$							
D95(d)	2.525(2.537)	3.466	3113	157.1	0.320	0.401	0.010
cc-pVTZ	2.497(2.508)	3.516	3892	161.1	...	0.390	0.004

[a] Potential energy curves were calculated at 25 points from 3.5 au to 26 au and were fit by the extended Rydberg function of order 8. D_e, ω_e, $\omega_e\chi_e$, B_e, and α_e are in cm^{-1}.

[b] K.P. Huber and G. Herzberg, "Molecular spectra and molecular structure. IV. Constants of diatomic molecules. (Van Nostrand,Princeton, 1979).

Input 645 ### SAC-CI SD-R for high-spin states

1. SAC-CI NV and V calculations are done for the high-spin states; quartet, quintet, sextet, and septet states of N_2, together with for singlet, triplet, cation doublet, anion doublet and triplet states for comparison.
2. D95 basis plus 1s Rydberg function is used and the dimension of AO basis is 22. The active space is limited as 5 occupied and 8 unoccupied MOs for comparison with the full-CI results.
3. Results of the SAC-CI SD-R NV and V without perturbation selection are well compared with the full-CI ones.
4. Results are improved by the general-R method for the two-electron excited states (states whose errors are larger than 11 mhartree in the SD-R calculations) as shown below in Input 646, though the computational labor increases in the general-R method (see Table 24, for example).
   Reference: H. Nakatsuji and M. Ehara, J. Chem. Phys. 98, 7179 (1993).

Table 23. Energies (in au) of the singlet to septet states of N_2 (R=1.09768 A) calculated by the SAC-CI SD-*R* method.

	SAC-CI-V	Δ(mH)	SAC-CI-NV	Δ(mH)	full-CI
Singlet states					
Σ_g^+	-108.54462	-5.15	-108.54351	-4.04	-108.53947

Δ_g	-108.27285	49.95	-108.27284	49.96	-108.32280
Π_g	-108.63761	1.14	-108.63711	1.64	-108.63875
Σ_u^-	-108.58847	6.62	-108.58832	6.77	-108.59509
Δ_u	-108.57735	9.41	-108.57712	9.64	-108.58676
Π_u	-108.48071	6.39	-108.48000	7.10	-108.48710
average discrepancy		13.11		13.19	
Triplet states					
Σ_g^+	-108.55950	-5.45	-108.55861	-4.56	-108.55405
Δ_g	-108.29989	11.43	-108.29989	11.43	-108.31132
Π_g	-108.68386	1.54	-108.68340	2.00	-108.68540
Δ_u	-108.63142	5.47	-108.63128	5.61	-108.63689
Σ_g^+	-108.67863	2.91	-108.67848	3.06	-108.68154
Π_u	-108.56275	2.56	-108.56210	3.21	-108.56531
average discrepancy		4.89		4.97	
CationDoublet states					
Σ_g^+	-108.43598	-6.11	-108.43497	-5.10	-108.42987
Σ_g^-	-108.76356	115.86	-107.76356	115.86	-107.87942
Π_g	-107.98665	94.92	-107.98665	94.92	-108.08157
Σ_u^-	-107.91474	95.69	-107.91474	95.69	-108.01043
Σ_u^+	-108.30916	-1.19	-108.30773	0.24	-108.30797
Π_u	-108.35714	3.99	-108.35687	4.26	-108.36113
average discrepancy		52.96		52.68	
Electron-attached states					
Σ_g^+	-108.90796	2.81	-108.90777	3.00	-108.91077
Σ_g^-	-108.54181	16.09	-108.54181	16.09	-108.55790
Π_g	-108.84493	10.84	-108.84477	11.00	-108.85577
Δ_u	-108.54533	16.31	-108.54533	16.31	-108.56164
Σ_u^+	-108.90480	2.03	-108.90456	2.27	-108.90683
Π_u	-108.56177	48.06	-108.56177	48.06	-108.60983
average discrepancy		16.02		16.12	
Quartet states					
Σ_u^+	-108.12523	0.25	-108.12455	0.93	-108.12548
Δ_u	-108.07536	3.25	-108.07512	3.49	-108.07861
Π_u	-108.05517	6.66	-108.05492	6.91	-108.06183
Σ_u^-	-108.04889	7.41	-108.04861	7.69	-108.05630
Π_g	-108.02199	2.41	-108.02176	2.64	-108.02440
Σ_g^+	-108.01252	3.50	-108.01206	3.96	-108.01602
Δ_g	-107.96190	5.52	-107.96161	5.81	-107.96742
Σ_g^-	-107.93785	9.85	-107.93756	10.14	-107.94770
average discrepancy		3.74		5.20	
Quintet states					
Π_u	-108.40170	0.78	-108.40158	0.90	-108.40248
Σ_g^+	-108.38212	-0.79	-108.38202	-0.69	-108.38133
Σ_u^-	-108.36682	5.50	-108.36671	5.61	-108.37232
Π_g	-108.29169	2.12	-108.29157	2.24	-108.29381
Σ_u^+	-108.25457	0.37	-108.25430	0.64	-108.25494
Σ_g^+	-108.21971	0.65	-108.21941	0.95	-108.22036
Δ_u	-108.20512	2.90	-108.20493	3.09	-108.20802
Π_u	-108.18053	6.62	-108.18032	6.83	-108.18715
Δ_g	-108.16981	3.12	-108.16959	3.34	-108.17293
Π_g	-108.15217	4.66	-108.15198	4.85	-108.15683
average discrepancy		2.59		2.78	

Sextet states					
Π_g	-107.81923	0.37	-107.81908	0.52	-107.81960
Σ_g^+	-107.80020	1.19	-107.80009	1.30	-107.80139
Σ_u^+	-107.69016	0.86	-107.69003	0.99	-107.69102
average discrepancy		0.81		0.94	
Septet states					
Σ_u^+	-107.90323	0.57	-107.90312	0.68	-107.90380

Table 24. Dimensions of SAC-CI and full-CI for singlet to septet states of N_2 (R=1.09768 A); SD-*R* without selection and general-*R* with selection.

	SD-*R*	general-*R*	full-CI
Singlet			
Σ_g^+, Δ_g	147	2430	54799
Σ_g^-, Δ_g	84	949	53002
Π_g	105	1514	53588
Σ_u^-, Δ_u	84	1131	52952
Σ_u^+, Δ_u	126	1865	54224
Π_u	105	1269	53638
Triplet			
Σ_g^+, Δ_g	146	2129	91862
Σ_g^-, Δ_g	116	1021	91874
Π_g	141	1151	92068
Σ_u^-, Δ_u	120	756	91864
Σ_u^+, Δ_u	162	653	92272
Π_u	137	1076	92078
Ionized			
Σ_g^+, Δ_g	36	1889	54244
Σ_g^-, Δ_g	16	1318	53152
Π_g	25	744	53633
Σ_u^-, Δ_u	16	1106	53192
Σ_u^+, Δ_u	35	1900	54179
Π_u	26	741	53698
Electron-attached			
Σ_g^+, Δ_g	54	492	123520
Σ_g^-, Δ_g	28	1092	121940
Π_g	41	1614	122630
Σ_u^-, Δ_u	28	1207	121840
Σ_u^+, Δ_u	54	444	123420
Π_u	41	1215	122730
Quartet			
Σ_g^+, Δ_g	228	873	44288
Σ_g^-, Δ_g	224	1146	44864
Π_g	234	750	44656
Σ_u^-, Δ_u	232	1030	44944
Σ_u^+, Δ_u	236	961	44368
Π_u	226	810	44576
Quintet			
Σ_g^+, Δ_g	584	1490	48775
Σ_g^-, Δ_g	608	1186	48985
Π_g	596	802	48770
Σ_u^-, Δ_u	612	1889	48980
Σ_u^+, Δ_u	580	1542	48560

Π_u	592	1119	48775
Sextet			
Σ_g^+	482	258	14732
Π_g	487	215	14599
Σ_u^+	478	202	14677
Septet			
Σ_u^+	772	380	11648

Input 646 ### SAC-CI general-R calculation

1. SAC-CI general-*R* calculations are done for the singlet to septet states of N_2 with LevelThree.
2. D95 basis plus 1s Rydberg function is used and the dimension of AO basis is 22. The active space is limited as 5 occupied and 8 unoccupied MOs for comparison with the full-CI results.
3. For generating higher-order operators, exponential-generation algorithm is used. FullRGeneration, in which all the higher operator before perturbation selection, is also available.

Reference : H. Nakatsuji and M. Ehara, J. Chem. Phys. 98, 7179 (1993).

Table 25. Energies (in au) of the singlet to septet states of N_2 (R=1.09768 A) calculated by the SAC-CI general-R method.

	SAC-CI-V general-*R*	Δ(mhartree)	full-CI (hartree)
Singlet states			
Σ_a^+	-108.53352	5.95	-108.53947
Δ_a	-108.31499	7.81	-108.32280
Π_a	-108.63389	4.86	-108.63875
Σ_a^-	-108.59372	1.37	-108.59509
Δ_u	-108.58258	4.18	-108.58676
Π_u	-108.48417	2.93	-108.48710
average discrepancy		4.52	
Triplet states			
Σ_a^+	-108.55280	1.25	-108.55405
Δ_a	-108.30724	4.08	-108.31132
Π_a	-108.68386	1.54	-108.68540
Δ_u	-108.63450	2.39	-108.63689
Σ_u^+	-108.67860	2.94	-108.68154
Π_u	-108.56296	2.35	-108.56531
average discrepancy		2.43	
CationDoublet states			
Σ_a^+	-108.42900	0.87	-108.42987
Σ_a^-	-107.87092	8.50	-107.87942
Π_a	-108.07524	6.33	-108.08157
Σ_u^-	-108.00522	5.21	-108.01043
Σ_u^+	-108.30623	1.74	-108.30797
Π_u	-108.35885	2.28	-108.36113
average discrepancy		5.15	
Electron-attached states			
Σ_a^+	-108.90703	3.74	-108.91077
Σ_a^-	-108.54572	12.18	-108.55790
Π_a	-108.85298	2.79	-108.85577
Δ_u	-108.54946	12.18	-108.56164

Σ_u^+	-108.90335	3.48	-108.90683
Π_u	-108.59527	14.56	-108.60983
average discrepancy		8.22	
Quartet states			
Σ_u^+	-108.12440	1.08	-108.12548
Δ_u	-108.07755	1.06	-108.07861
Π_u	-108.05902	2.81	-108.06183
Σ_u^-	-108.05434	1.96	-108.05630
Π_g	-108.02149	2.91	-108.02440
Σ_g^+	-108.01471	1.31	-108.01602
Δ_g	-107.96637	1.05	-107.96742
Σ_g^-	-107.94635	1.35	-107.94770
average discrepancy		1.69	
Quintet states			
Π_u	-108.40113	1.34	-108.40248
Σ_g^+	-108.38023	1.08	-108.38133
Σ_u^-	-108.37014	2.18	-108.37232
Π_g	-108.29197	1.83	-108.29381
Σ_u^+	-108.25334	1.44	-108.25494
Σ_g^+	-108.21896	1.34	-108.22036
Δ_u	-108.20656	1.28	-108.20802
Π_u	-108.18379	3.35	-108.18715
Δ_g	-108.17156	1.32	-108.17293
Π_g	-108.15289	3.94	-108.15683
average discrepancy		1.91	
Sextet states			
Π_g	-107.81833	1.27	-107.81960
Σ_g^+	-107.80072	0.67	-107.80139
Σ_u^+	-107.68979	1.23	-107.69102
average discrepancy		1.06	
Septet states			
Σ_u^+	-107.90297	0.83	-107.90380

Input 647 ### Geometry optimization with general-R

1. Geometry optimizations of the SAC-CI general-*R* and SD-*R* methods are performed for the $C'^1\Delta$ state of BH.
2. D95(d,p) basis set [4s2p1d/2s1p] is used and the dimension of AO basis is 21. The active space is full (3 occupied and 18 unoccupied MOs).
3. $C'^1\Delta$ state is described by the two-electron process, for which general-*R* method is more reliable than SD-*R* method.
4. The ground state is also optimized by the SAC with "SacOnly" to calculate T_0 (compared with exptl. T_e).
5. Details of the spectroscopic constants are given in the paper.

Reference: M. Ishida, K. Toyota, M. Ehara and H. Nakatsuji, *Chem. Phys. Lett.* 347, 493 (2001).

Table 26. Optimized structure and energy of the ground $X^1\Sigma_g^+$ and singlet $C'^1\Delta$ states of BH.

Method	Excitation	With selection (Input 647)	Without selection[a]

	level	R_e (A)	T_e / T_0 (eV)	Total energy(au)	R_e (A)	T_e / T_0 (eV)	Total energy(au)
$X^1\Sigma_g^+$							
SAC	0	1.244	---	-25.20581	1.243	---	(-25.21999)
Exptl.		1.232	---		1.232	---	
$C'^1\Delta$							
SD-*R*	2	1.190	6.772	-24.95579	1.190	6.815	(-24.96954)
general-*R*	2	1.200	6.137	-24.97951	1.198	6.092	(-24.99612)
Exptl.		1.196	5.701		1.196	5.701	

[a] M. Ishida, K. Toyota, M. Ehara and H. Nakatsuji, *Chem. Phys. Lett.* 347, 493 (2001); calculation without selection, total energies are given without final single point calculation after energy optimization.

Table 27. SAC-CI dimensions for the optimization of $X^1\Sigma_g^+$ and $C'^1\Delta$ states.

Method	With selection	Without selection
Singlet $X^1\Sigma_g^+$		
SAC	401	567
Singlet $C'^1\Delta$		
SAC-CI SD-*R*	95	228
general-*R*	376	3628

Input 648 ### Geometry optimization of high-spin states

1. Geometry optimizations of the SAC-CI DT-R and DTQ-R method are done for the $X^4\Sigma_g^-$ and $B^4\Sigma_u^-$ states of C_2^+.
2. D95(d) basis set [4s2p1d] is used and the dimension of AO basis is 32. The active space is full (6 occupied and 26 unoccupied MOs).
3. Results are improved by the DTQ-R method, especially for the adiabatic excitation energy (Te) of $B^4\Sigma_u^-$ state, since it is described by three-electron process.

Table 28. Geometry and energy of the $X^4\Sigma_g^-$ and $B^4\Sigma_u^-$ states of C_2^+ calculated by the SAC-CI method.

Method	Excitation level	D95(d) (Input 648)			cc-pVTZ without f [a]		
		R_e (A)	T_e / T_0 (eV)	Total energy(au)	R_e (A)	T_e / T_0 (eV)	Total energy(au)
$X^4\Sigma_g^-$							
DT-*R*	2	1.422	---	-75.27295	1.406	---	(-75.32047)
DTQ-*R*	2	1.419	---	-75.29285	1.407	---	(-75.33974)
Exptl.		1.403	---		1.403	---	
$B^4\Sigma_u^-$							
DT-*R*	3	1.342	5.328	-75.09474	1.323	5.125	(-75.13212)
DTQ-*R*	3	1.368	2.910	-75.19764	1.349	2.617	(-75.24358)
Exptl.		1.347	2.436		1.347	2.436	

[a] M. Ishida, K. Toyota, M. Ehara and H. Nakatsuji, Chem. Phys. Lett. 350, 351 (2001); calculation with better thresholds (EThreS2=EThreR2=EThreEgR=1.d-7, CThreULR1=CThreULR2=0.005), Total energies are given without final single point calculation after energy optimization.

Input 649 ### **Force at vertical excited states**

1. Internal coordinate forces in the singlet($n \to \pi^*$), triplet($n \to \pi^*$), and ionized states($n \to$) of HNO are calculated by the SAC-CI SD-*R* V method.
2. Dimension of AO basis is 22. The active space is full (8 occupied and 14 unoccupied MOs).
3. Molecular geometry is the SAC-optimized ground-state one, the force is the one at the vertical excited state. Therefore, this result indicates how the geometry changes in these excited and ionized states.
4. LevelThree is employed as the thresholds for the linked operators.

Table 29. Internal coordinate forces in S_1($n \to \pi^*$), T_1($n \to \pi^*$), and I_1 states($n \to$) of HNO.

State	Nature	Force (Hartree/Bohr or radian)	
S_1[c]	$n \to \pi^*$	dE/dR(NO)	0.0414
		dE/dR(NH)	-0.0062
		dE/dA(HNO)	0.0236
T_1	$n \to \pi^*$	dE/dR(NO)	0.0273
		dE/dR(NH)	-0.0136
		dE/dA(HNO)	0.0335
I_1	$n \to$	dE/dR(NO)	-0.0863
		dE/dR(NH)	0.0064
		dE/dA(HNO)	0.0418

[a] R(NO), R(NH), and A(HNO) denote NO bond length, NH bond length, and HNO bond angle, respectively.
[b] A positive sign means enlargement of bond length or angle.
[c] The following geometry changes according to $S_0 \to S_1$ excitation were observed:
dR(NO) =+0.030 (Ang.), dR(NH) =-0.026 (Ang.), and dA(HNO)=+7.7 (deg..).
(F.W. Dalby, Can. J. Phys. 36 (1958) 1336.)

Input 650 ### **H_2CO: Singlet, triplet, Ionized: All properties**

1. Singlet, triplet, ionized, and electron-attached states of H_2CO are calculated by the SAC-CI SD-*R* method.
2. cc-pVDZ plus Rydberg functions [1s1p] is used and the dimension of AO basis is 46. The active space is full-valence (6 occupied and 38 unoccupied MOs); 1s orbitals are frozen as core.
3. Density and Transition density are calculated as the expectation values.
4. All available properties (multipole moments, N-th moments, electrostatic properties, and diamagnetic terms) of the singlet triplet, ionized, and electron-attached states of H_2CO are calculated.

Table 30. Excitation energy, dipole moment, and oscillator strength of the singlet states of HCHO.

		Excitation energy (eV)		Dipole moment(au)		Oscillator Strength	
State	Character	SAC-CI	Exptl.	SAC-CI	Exptl.	SAC-CI	Exptl.
$1A_1$	ground	0.00		0.939	0.913		
$1A_2$	$n \to \pi^*$	4.18	4.1, 4.2	0.510	0.614	---	
$1B_2$	$n \to 3s$	7.01	7.091, 7.13	-1.131		0.0244	0.028
$2A_1$	$n \to 3p_y$	7.95	8.14	0.061		0.0561	0.017

$2B_2$	$n \to 3p_z$	7.95	7.97, 8.00	0.700	0.0443	0.032
$2A_2$	$n \to 3p_x$	8.19		0.303	---	
$3B_2$	$n \to 3s$	9.35		2.067	0.0148	
$3A_1$	$n \to 3p_y$	9.54		1.025	0.0449	
$1B_1$	$5a_1 \to \pi^*$	9.59		0.203	0.0013	
$3A_2$	$n \to 3p_x$	9.66		0.740	---	
$4A_1$	$\pi \to \pi^*$	10.33	10.7	0.087	0.1018	
$2B_1$	$\pi \to 3s$	10.84	10.7	-1.177	0.0410	
$3B_1$	$n \to 3p_z$	11.80	11.6-11.9	0.701	0.0390	

"---" : optically forbidden, $5a_1$: sigma

Table 31. Excitation energy and dipole moment of the triplet states of HCHO.

State	Character	Excitation energy (eV)		Dipole moment (au)	
		SAC-CI	Exptl.	SAC-CI	Exptl.
$1A_2$	$n \to \pi^*$	3.71	3.5, 3.3-3.6	0.461	0.508
$1A_1$	$\pi \to \pi^*$	6.11	6.0, 5.6-6.2	0.329	
$1B_2$	$\pi \to 3s$	6.85	7.09, 6.7-7.0	-1.189	
$2B_2$	$n \to 3p_z$	7.82	7.92	1.132	
$2A_1$	$n \to 3p_y$	7.85	8.11	-0.063	
$2A_2$	$n \to 3p_x$	8.22		0.182	
$1B_1$	$5a_1 \to \pi^*$	8.69	8.50	0.113	
$3B_2$	$\pi \to 3s$	9.30		0.818	
$3A_1$	$n \to 3p_y$	9.45		1.258	
$3A_2$	$1b_2 \to \pi^*$	10.43		1.210	
$2B_1$	$\pi \to 3s$	10.78		-0.924	
$3B_1$	$n \to 3p_z$	11.66		0.405	

1b2: sigma

Table 32. Ionization Potential of HCHO.

State Character	Character	Ionization Potential (eV)	
		SAC-CI	Exptl.
$1B_2$	n	10.47	10.9
$1B_1$	π	14.33	14.5
$1A_1$	$5a_1$	15.80	16.2
$2B_2$	$1b_2$	17.14	17.0
$2A_1$	$4a_1$	21.34	21.15 ± 0.15

Table 33. Second moment and diamagnetic susceptibilities of the singlet states of HCHO.

State	Character	Second moment (au)				Diamagnetic Susceptibilities			
		$< x^2 >$	$< y^2 >$	$< z^2 >$	$< r^2 >$	x^2	y^2	z^2	r^2
$1A_1$	ground	8.8	15.3	37.2	61.3	78.8	69.0	36.1	183.9
$1A_2$	$n \to \pi^*$	10.6	14.3	37.2	62.0	77.1	71.6	37.3	186.0
$1B_2$	$\pi \to 3s$	20.2	26.2	48.9	95.3	112.6	103.7	69.7	286.0
$2A_1$	$n \to 3p_y$	18.7	46.1	45.8	110.5	137.8	96.7	97.1	331.6

$2B_2$	$n \to 3p_z$	20.7	25.4	65.4	111.4	136.1	129.1	69.1	334.3
$2A_2$	$n \to 3p_x$	43.3	24.2	46.0	113.6	105.3	134.0	101.3	340.7
$3B_2$	$n \to 3s$	17.7	22.6	80.4	120.7	154.6	147.2	60.5	362.2
$3A_1$	$n \to 3p_y$	16.7	39.0	54.9	110.6	140.9	107.4	83.7	331.9
$1B_1$	$5a_1 \to \pi^*$	10.4	15.2	36.3	61.9	77.3	70.1	38.4	185.8
$3A_2$	$n \to 3p_x$	41.1	23.5	58.9	123.5	123.6	150.0	96.8	370.4
$4A_1$	$n \to \pi^*$	13.4	24.4	43.8	81.6	102.2	85.8	56.7	244.7
$2B_1$	$\pi \to 3s$	18.9	27.1	49.4	95.4	114.7	102.4	69.0	286.1
$3B_1$	$n \to 3p_z$	19.7	26.4	65.8	111.9	138.3	128.2	69.3	335.8

Gauge origin (0.00 0.00 0.00)

Table 34. Second moment and diamagnetic susceptibilities of the triplet states of HCHO.

State	Character	Second moment (au)				Diamagnetic Susceptibilities			
		$< x^2 >$	$< y^2 >$	$< z^2 >$	$< r^2 >$	x^2	y^2	z^2	r^2
$1A_2$	$n \to \pi^*$	10.6	14.2	37.0	61.8	76.8	71.4	37.2	185.4
$1A_1$	$\pi \to \pi^*$	9.1	15.3	37.8	62.2	79.7	70.4	36.6	186.7
$1B_2$	$\pi \to 3s$	18.8	25.4	48.4	92.6	110.7	100.7	66.3	277.7
$2B_2$	$n \to 3p_z$	19.8	24.5	61.4	105.6	128.8	121.7	66.4	316.8
$2A_1$	$n \to 3p_y$	18.1	44.6	45.6	108.2	135.2	95.5	93.9	324.6
$2A_2$	$n \to 3p_x$	43.8	24.4	46.2	114.4	105.9	135.0	102.2	343.1
$1B_1$	$5a_1 \to \pi^*$	10.2	15.2	36.1	61.5	76.9	69.5	38.1	184.5
$3B_2$	$\pi \to 3s$	17.4	22.9	79.6	119.9	153.8	145.4	60.4	359.7
$3A_1$	$n \to 3p_y$	17.7	42.7	57.6	117.9	150.4	112.8	90.5	353.8
$3A_2$	$1b_2 \to \pi^*$	11.1	14.0	37.8	62.9	77.6	73.4	37.7	188.7
$2B_1$	$\pi \to 3s$	18.6	26.8	48.1	93.4	112.3	99.9	68.0	280.2
$3B_1$	$n \to 3p_z$	18.1	24.9	63.1	106.0	131.9	121.7	64.4	318.0

Input 651 ### H_2CO Geometry opt. for singlet & triplet states

1. Geometry optimization is performed for the ground and singlet A" excited states of HCHO by the SAC/SAC-CI SD-R method. Initial guess geometry is the experimental one.
2. DZ1P[4s2p1d/2s] basis set is used and the dimension of AO basis is 36. The active space is full (8 occupied and 28 unoccupied MOs)
3. MacroIter=1 (default) is used: one cycle of optimization with perturbation selection at initial geometry and an additional single-point SAC/SAC-CI calculation.
4. The MOD (minimum-orbital deformation) method with the canonical MOs (CMOs) at the initial geometry is used (default).

Table 35. Optimized structure and energy of the ground and the lowest singlet A" and triplet A" excited states of HCHO.

Method	R(HC) (A)	R(CO) (A)	$\angle HCH$ (degree)	$\angle OOP$ [a]	T_e / T_0 [b] (eV)	Total energy (au)
X^1A' ground state						
SAC-CI	1.109	1.217	116.4	-	-	-114.19176
Exptl.	1.101	1.203	116.3	0.0	-	-

A^1A'' singlet excited state						
SAC-CI	1.099	1.325	118.1	38.80	2.979	-114.05166
Exptl.	1.097	1.321	118.6	31.75	3.495	-
a^1A'' triplet excited state						
SAC-CI	1.102	1.314	116.0	46.44	2.398.	-114.06786
Exptl.	1.10	1.28	116	38	3.124	-

[a] Out of plane.
[b] Theoretical adiabatic excitation energy is given by T_e and experimental one by T_0.

Input 652 ### Hyperfine Splitting Constants

1. Hyperfine splitting constants (hfsc) of CH_3, H_2O^+, and NH_2 radicals are calculated.
2. D95 basis sets are used and the dimension of AO basis is 16, 14, and 14 for CH_3, H_2O^+, and NH_2, respectively. All SCF MOs are included in the active space (default for SpinDensity).

Table 36. Hfsc of samll radicals calculated by the SAC-CI SD-R method.

Molecule	State	Total energy (au)	Atom	hfsc(Gauss)		
				SAC-CI		Exptl.
				GTO[a]	STO[b]	
CH_3^+	A_2''	-39.65860	C	32.4	25.6	28.7
			H	-27.9	-29.6	-24.7
H_2O^+	B_1	-75.73233	O	-22.2	-26.0	-29.7
			H	-28.1	-24.1	-26.1
NH_2	B_1	-55.66341	N	8.0	7.3	9.95
			H	-24.9	20.1	-24.12

[a] Input 652
[b] H. Nakatsuji, M. Izawa, J. Chem. Phys. 91, 6205 (1989)
H. Nakatsuji, M. Izawa, J. Chem. Phys. 97, 435 (1992)
Thresholds and algorithm for calculating spin density are different from these references.

Input 653 ### Separation of electron repulsion integral

1. Allocation of the electron repulsion integrals all-in-one or separately.
2. Singlet V state and 3d Rydberg state of pyrrole are calculated by the SAC-CI SD-R method with 6-311+G(2d,p) for N and C and 6-31G(d,p) for H
3. Dimension of AO basis is 160 and the active space is full-valence (13 occupied and 142 unoccupied MOs).
4. For the machines with small core memory, electron repulsion integrals (ERI) are separately allocated in memory and disc. In this sample, core memory of 50MB and 200MB is used; the former job separates the ERI into 4 unit, while the latter does not separate.

Table 37. Dimension and CPU time of the SAC-CI calculations for the singlet V and 3d Rydberg states of pyrrole.

State	Dimension	Character	E (eV)	Oscillator strength
Ground	17138		---	---
Excited A_1	19818	V	6.321	0.0000
		3d Rydberg	7.570	0.0617
CPU time (sec)	Separated		Non-separated	
Total	33m34s		21m39s	

Input 689 ### Geometry optimization and numerical frequency

1. Numerical frequency calculation of the SAC-CI SD-*R* method is performed for the A" excited state of HCF.
2. D95 basis set [4s2p/2s] is used and the dimension of AO basis is 22. The active space is full (8 occupied and 14 unoccupied MOs).
3. Before geometry optimization, GSUM method is performed for the structures in the vicinity of equilibrium structure.
4. Effect of polarization function is shown in the table.

Table 38 Spectroscopic parameters of the ground and excited states of HCF.

	ground A'			excited A"		
	SAC-CI		Exptl.	SAC-CI		Exptl.
	D95 (test689)	D95(d)		D95 (test689)	D95(d)	
Structure parameter						
R_{CF} (Å)	1.412	1.322	1.305	1.384	1.314	1.308
R_{HC} (Å)	1.143	1.126	1.138	1.116	1.105	1.063
<HCF(°)	100.6	102.1	104.1	124.1	123.8	123.8
Adiabatic excitation energy (eV)						
	-	-	-	2.31	2.36	2.142
Harmonic frequency (cm^{-1})						
	1075	1208		998	1074	1021
	1368	1447	1403	1121	1367	
	3062	2787		2941	3062	

Input 921 ### Free-Base Porphin using direct algorism

The singlet excited states of free-base porphin with Huzinaga double zeta basis and LevelThree threshold. The Q bands (the lowest states) were well described by the SAC-CI method. The excitation energy of the B band was overestimated about 0.3 eV.

Table 39. Singlet excited states of free-base porphin

	SAC-CI				Exp. (eV)
State	Main configuration	Nature	E_{ex}(eV)	f (au)	
$1B_{3u}$	$(4b_{3u}\rightarrow 3b_{2g})$-$(1a_u\rightarrow 4b_{1g})$	$\pi\rightarrow\pi^*$	1.86	0.000	1.98 (Q_x: very weak)
$1B_{2u}$	$(4b_{3u}\rightarrow 4b_{1g})$-$(1a_u\rightarrow 3b_{2g})$	$\pi\rightarrow\pi^*$	2.46	0.000	2.42 (Q_y: very weak)
$2B_{3u}$	$(1a_u\rightarrow 4b_{1g})$+$(4b_{3u}\rightarrow 3b_{2g})$-$(3b_{3u}\rightarrow 3b_{2g})$	$\pi\rightarrow\pi^*$	3.62	1.371	3.33 (B: Strong)
$2B_{2u}$	$(1a_u\rightarrow 3b_{2g})$-$(4b_{3u}\rightarrow 4b_{1g})$	$\pi\rightarrow\pi^*$	3.73	1.786	3.65 (N: broad)
$3B_{3u}$	$(3b_{3u}\rightarrow 3b_{2g})$-$(4b_{3u}\rightarrow 3b_{2g})$	$\pi\rightarrow\pi^*$	4.23	0.641	
$1B_{1u}$	$(16b_{2u}\rightarrow 4b_{1g})$	$n\rightarrow\pi^*$	4.45	0.004	4.25-4.67 (L: weak)
$3B_{2u}$	$(3b_{3u}\rightarrow 4b_{1g})$+$(2b_{3u}\rightarrow 4b_{1g})$	$\pi\rightarrow\pi^*$	4.47	0.210	
$4B_{2u}$	$(2b_{3u}\rightarrow 4b_{1g})$	$\pi\rightarrow\pi^*$	4.98	0.389	5.0-5.5 (M: weak)
$4B_{3u}$	$(2b_{3u}\rightarrow 3b_{2g})$	$\pi\rightarrow\pi^*$	5.11	0.484	

Input 922 ### H_2CO Geometry opt. for singlet & triplet states using direct algorism

Ground and excited states geometries and adiabatic transition energies of formaldehyde with D95(d) basis and LevelThree threshold. The planar ground state and non-planar excited states were

well reproduced by the SAC-CI method. The calculated adiabatic transition energies agreed well with the experimental 0-0 transition energies.

Table 40. Optimized structures and transition energies of formaldehyde.

Method	Geometry (angstrom and degree)				T_e/T_0[b]	Total energy
	R(HC)	*R*(CO)	<HCH	OOP.[a]	(eV)	(E_h)
X^1A' ground state						
SAC	1.109	1.219	116.5	0		-114.196803
Experiment	1.101	1.203	116.3	0		
$1^1A''$ singlet excited state						
SAC-CI	1.100	1.333	119.3	29.43	3.554	-114.066184
Experiment	1.097	1.321	118.6	31.75	3.495	
$1^1A''$ triplet excited state						
SAC-CI	1.102	1.322	116.8	38.84	3.103	-114.082757
Experiment	1.10	1.28	116	38	3.124	

[a]out-of plane angle.
[b]Theoretical adiabatic transition energies are given by T_e and the experimental values are T_0.

Input 923 ### Separation of electron repulsion integral using direct algorism

Excitation, ionization, and electron attachment energies of pyrrole with 6-311+G** basis in LevelThree accuracy. Valence pi-pi* excited states strongly mix with the Rydberg states and therefore, diffuse functions are necessary for describing the pi-pi* excited states. Additional Rydberg basis sets were required for the calculations of Rydberg states.

Table 41. Excitation, ionization, and electron-attachment energies of pyrole.

State	Nature	Eex(eV)[a]	Osc.(au)[b]	Exp.
Singlet states				
1^1A_2	$\pi_3\rightarrow$diffuse	5.27	0.000	
1^1B_1	$\pi_3\rightarrow$diffuse, $\pi_2\rightarrow$diffuse	6.12	0.035	6.2~6.5
1^1B_2	$\pi_3\rightarrow(\pi_4^*$, diffuse)[c]	6.25	0.213	
1^1A_1	$\pi_2\rightarrow(\pi_4^*$, diffuse), $\pi_3\rightarrow(\pi_5^*$, diffuse)	6.39	0.000	
2^1A_1	$\pi_2\rightarrow(\pi_4^*$, diffuse), $\pi_3\rightarrow(\pi_5^*$, diffuse)	7.60	0.013	7.5~8.0
Triplet states				
1^3B_2	$\pi_3\rightarrow(\pi_4^*$, diffuse)	4.39		4.20
1^3A_2	$\pi_3\rightarrow$diffuse	5.27		
1^3A_1	$\pi_2\rightarrow(\pi_4^*$, diffuse), $\pi_3\rightarrow(\pi_5^*$, diffuse)	5.53		5.10
1^3B_1	$\pi_3\rightarrow$diffuse, $\pi_2\rightarrow$diffuse	6.07		
Caton doublet states				
1^2A_2	$1a_2(\pi_3)^{-1}$	7.98	0.931	8.02, 8.21
1^2B_1	$2b_1(\pi_2)^{-1}$	8.82	0.921	9.05, 9.20
1^2A_1	$9a_1(\sigma)^{-1}$	12.73	0.906	12.58, 12.60
1^2B_2	$6b_2(\sigma)^{-1}$	13.18	0.908	13.0
Anion doublet states				
1^2A_1	$10a_1$(diffuse)$^{+1}$	1.30		
1^2B_2	$7b_2$(diffuse)$^{+1}$	1.92		
1^2B_1	$3b_1(\pi_4^*)^{+1}$[c]	2.54		2.36
1^2A_2	$1a_2(\pi_5^*)^{+1}$	3.74		3.45

[a]Excitation energies for excited states, vertical ionization energies for cation doublet states, and vertical electron attachment energies for anion doublet states.
[b]Monopole intensities for cation doublet states.

[c]Diffuse functions mix strongly to the valence pi* orbital.

Input 924 ### Geometry optimization and numerical frequency using direct algorism

Geometries and vibrational frequencies of fluoromethylene (HCF) molecule in the ground and lowest singlet excited states. D95(d,p) basis set was used. The GSUM method was used to ensure the smoothness of the potential surfaces.

Table 42

Method	Geometry (angstrom and degree)			Freqency (cm^{-1})		
	R(CF)	*R*(CH)	<HCF	CF stretch	bend	CH stretch
X^1A' ground state						
SAC	1.325	1.130	102.6	1272	1459	2919
Experiment	1.305	1.138	104.1		1403	
$1^1A''$ excited state						
SAC-CI	1.321	1.102	123.9	1161	1328	3125
Experiment	1.308	1.068	123.8	1021		

Input 925 ### Circular dichroism spectrum of R-methyloxirane

Circular dichroism of R-methyloxirane with the direct SAC-CI code. The basis functions employed were cc-pVTZ sets plus double Rydberg functions for C, O, and H atoms of the three-membered ring and cc-pVDZ sets for the methyl group. The gauge origin is at the center of gravity. The rotatory strengths of the CD spectra were calculated using both the length and velocity forms. The former is gauge-origin dependent, but the latter is not, and so the latter is more reliable for large molecules.

Table 43. Singlet excited states of R-methyloxirane

SAC-CI				length	velocity	Exp.	
State	Nature	E_{ex}(eV)	f (au)	$R_{len}(10^{-40}$cgs)[a]	$R_{vel}(10^{-40}$cgs)[b]	E_{ex}(eV)	R(10^{-40}cgs)
1^1A	n(O)→3s	7.02	0.009	–10.253	–10.974	7.08	–12.5
2^1A	n(O)→3p	7.42	0.010	–0.896	–1.016		
3^1A	n(O)→3p	7.48	0.016	5.355	5.238	7.70	+5.9
4^1A	n(O)→3p	7.67	0.011	1.898	2.108		
5^1A	σ→3s	7.85	0.004	6.644	7.742		
6^1A	σ→3p	8.39	0.005	–0.826	–1.809		
7^1A	σ→3p	8.44	0.029	–9.971	–8.976	8.35	–4.1
8^1A	σ→3p	8.52	0.002	–4.698	–4.954		
9^1A	n(O)→3d	8.64	0.006	1.159	1.288		

[a]Rotataory strength using length form
[b]Rotatory strength using velocity form

Input 965 ### O1s core ionized state of H_2O and N1s core ionized states of N_2

1. The O1s core-hole state of H_2O and N1s core-hole states ($1\sigma_g^{-1}$ and $1\sigma_u^{-1}$) of N_2 are calculated by the direct SAC-CI SD-*R* V method.
2. The cc-pVTZ basis set [4s3p2d1f/3s2p1d] is used and the AO dimensions are 58 and 60 in the calculations of H_2O and N_2, respectively.
3. **CorePrWindow** option activates the calculation of core-electron processes and specifies the range of core orbitals (*m*~*n*) with **CorePrWindow=(*m, n*)**. In the molecules with some equivalent atoms, core-orbitals of all atoms should be specified.

ex.) CorePrWindow=(1,1) for H_2O, and CorePrWindow=(1,2) for N_2.

Table 44. Direct SAC-CI SD-*R* Variational calculation of the core ionization energy (eV) for H_2O and N_2 with cc-pVTZ basis.

State	SAC-CI	Expt.
H_2O		
$O1s^{-1}$	540.433	539.79 [a]
N_2		
$N1s^{-1}\ \Sigma_u$	410.429	409.83 [b]
$N1s^{-1}\ \Sigma_g$	410.529	409.92 [b]
g-u splitting	0.100	0.097 [b]

[a] R. Sankari, M. Ehara, H. Nakatsuji, K. Ueda *et al.*, Chem. Phys. Lett. 380, 647 (2003)
[b] Adiabatic values including zero-point energy; M. Alagia, R. Richter, S. Stranges *et al.*, Phys. Rev. A 71, 012506 (2005).

Input 966 ### C1s-π* and O1s-π* core excited states of CO

1. C1s-π* and O1s-π* core excited states of CO are calculated by the direct SAC-CI SD-*R* V method.
2. The cc-pVTZ basis set [4s3p2d1f] is used and the AO dimension is 60.
3. The CorePrWindow is set as (1,1) and (2,2) for calculating O1s-π* and C1s-π* core excited states, respectively. The separate calculations are necessary for obtaining O1s-π* core excited state. The CorePrWindow=(1,2) calculation with many solutions provides numerous C1s core excited states, but not O1s core excited state.

Table 45. Direct SAC-CI SD-*R* calculation for C1s and O1s core excitation energy (eV) of CO with cc-pVTZ basis.

State	SAC-CI	Expt.
CO		
$C1s^{-1}$	287.66	287.41 [a]
$O1s^{-1}$	535.11	~ 534.5 [b]
		533.57 [c]

[a] S.J. Osborne, A. Ausmees, S. Svensson *et al.*, J. Chem. Phys. 102, 7317 (1995)
[b] Vertical excitation energy estimated by the peak maximum of vibrational spectrum; R. Püttner, I. Dominguez, T. J. Morgan *et al.*, Phys. Rev. A 59, 3415 (1999).
[c] Adiabatic excitation energy

Part II. Program Explanation and Namelist Input Manual for SAC/SAC-CI Program

II-A. SAC and SAC-CI SD-*R* Part (Main Steps) (See Table 1 of Part I-D-1)

* Step to control SAC/SAC-CI Program *

#SUPER97#

Note: Step name is bracketed by two "#" like #SUPER97#.

Namelist Group -- &CNTL --

This namelist group gives the information for controlling the job stream of the SAC/SAC-CI calculations and is given in the "keyword" form explained below.

Note that these "keywords" are different from the "Keyword Input" of Gaussian, but, are defined under the namelist input &CNTL.

The keywords must be written between "&CNTL" and "&END". The keywords consists of main keywords and sub keywords. The sub keywords must be written after its main keyword with parentheses, for example,

&CNTL SINGLET(SAC-CI-NV PROPERTY) IONIZED(GENERAL-R) &END

==========

TITLE : Title of calculation must be given as sub keyword in parenthesis. 80 characters from the beginning of sub keyword are effective.

Sub keywords

Title of calculation

Usage

&CNTL TITLE(Free Base Porphin SAC-CI) &END

==========

NONHF : Calculate fock matrix, when non-canonical orbitals are used as reference orbitals. Step #FOCK# is necessary.

See #FOCK#.

Sub keywords none

Default Hartree-Fock canonical orbitals are used as be reference orbitals.

Usage

&CNTL NONHF &END

==========

SINGLET : Calculate singlet states.
TRIPLET : Calculate triplet states.
IONIZED : Calculate doublet ionized states.
ANIONIZED : Calculate doublet electron-attached states.
QUARTET : Calculate quartet ionized states.
QUINTET : Calculate quintet states.
SEXTET : Calculate sextet ionized states.
SEPTET : Calculate septet states.

Sub keywords

Choice of the method

SAC-CI : Do SAC/SAC-CI method (Default). All sub-keywords below are acceptable.
SD-CI : Do only SD-CI method. Only the sub-keywords, ITERATIVE and DIRECT, are acceptable.
S-CI : Do only S-CI method. No sub-keywords below are available.

Choice of the range of the excitation operators

SD-*R* : SAC/SAC-CI SD-*R* method (Default)
GENERAL-*R* : SAC/SAC-CI general-*R* method

Choice of property calculations of SAC/SAC-CI wave function

PROPERTY : Calculate one electron property for the SAC/SAC-CI wave functions.
TRANS : Calculate transition moment.
HFSC : Calculate hfsc and cusp values for the SAC-CI wave functions for doublet, triplet, quartet, quintet, sextet, and septet states.
(Default: TRANS)

Choice of secular equation

SAC-CI-V : Solve SAC-CI-V (See ref. c-4) equation. Program uses the step sciv or das.
SAC-CI-NV : Solve SAC-CI-NV (See ref. c-4) equation. Program uses the step scinv or dnas.
(Default: SAC-CI-V)

Choice of method for linear-equation and diagonalization(See Table below)

ITERATIVE : Iterative procedure. Program uses the step sac, sciv or scinv.
DIRECT : InCoreDirect procedure. Program uses the step dsac, das, or dnas.
(Default: ITERATIVE)

Table. Correspondence between sub-keywords and steps for the SAC/SAC-CI method and CI method.

	SAC-NV	SAC-CI-V	SAC-CI-NV	CI
ITERATIVE	sac	sciv	scinv	cid
DIRECT	dsac	das	dnas	das

Choice of initial vector for iterative diagonalization

For singlet, triplet, ionized, and electron-attached states

S-INITIAL : S(Single excitation)-CI wave function
SD-INITIAL: SD(Single and double excitation)-CI wave function
(Default: SD-INITIAL)

For quartet and quintet states
D-INITIAL : D(double excitation)-CI wave function
DT-INITIAL: DT(Double and triple excitation)-CI wave function
(Default: DT-INITIAL)

For sextet and septet states
T-INITIAL : T(Triple excitation)-CI wave function
TQ-INITIAL: TQ(Triple and quadruple excitation)-CI wave function
(Default: TQ-INITIAL)

Default
Calculate SAC-NV and SAC-CI-V method by iterative procedure with SD(or DT,TQ)-CI vectors as initial guess.
Transition property is calculated.

Usage

1. SAC-CI SD-*R* for singlet states with SAC-CI-V method by iterative diagonalization using S-CI vector as initial guess. One electron properties are calculated.

```
&CNTL    SINGLET(S-INITIAL PROPERTY)    &END
```

2. SAC-CI general-*R* for ionized states with SAC-CI-NV method by incoredirect diagonalization.

```
&CNTL    IONIZED(GENERAL-R SAC-CI-NV DIRECT)    &END
```

3. SAC-CI SD-*R* for quartet states with SAC-CI-NV method by iterative diagonalization using D-CI vector as initial guess. Hfsc calculation is followed.

```
&CNTL    QUARTET(SAC-CI-NV D-INITIAL HFSC)    &END
```

==========

RESTART : Restart calculation. When restart keyword is added to the input data of terminated job, the calculation restart from the step terminated in the previous calculation.

Sub keywords none

Usage

When the job with the input

```
&CNTL    SINGLET    &END
```

is terminated, the restart should be done with the input

```
&CNTL    SINGLET  RESTART    &END
```

OUTPUT(O) file information

ifsccm(O)

##

---

* Step before pres * #BPRES#

In this step, some jobs necessary before PRES are done.

(1) MO Electron Repulsion Integrals (MOERIs) made in previous Overlay (Overlay 8) are sorted in a SAC/SAC-CI adapted form with molecular symmetry.
(2) Molecular symmetry used in the SAC/SAC-CI steps is specified.
(3) Step #FOCK# is called, if necessary.
(4) Initial sizes of the SAC/SAC-CI arrays are defined.

Input

Namelist group -&BPRES-

SYMERI

```
SYMERI =0:    Use molecular symmetry of Gaussian.
       =1:    Do not use symmetry.
       =2:    Use symmetry specified by namelist.
       (Default: 0)
```

SYM

```
Point group of molecule.
       = 'C1 ', 'C2V', ... etc (when symeri=2)
       (Default: Transferred from Gaussian)
```

MOS

```
Number of irreducible representation.
       = n1, n2, n3, ...
See step #PRES# for details.
(Default: Transferred from Gaussian)
```

IPRINT

```
Level of printing, see &PRES for details.
(Default: 0)
```

Sample input

```
&BPRES    SYMERI=2, SYM='Cs',
          MOS= 1, 1, 2, 1, 2, 2, 1,      &END
```

OUTPUT(O) file information

ifscmo(O), ifscer(O), ifscfi(O), ifscsi(O)

##

* Step Prescription * #PRES#

In this step,

(1) We define linked excitation operators (Symmetry-Adapted Linked Cluster Generators) at the singles and doubles level for each symmetry of

singlet states,
triplet states,
doublet ionized states,
doublet electron-attached (anion) states,
quartet ionized states,
quintet states,
sextet ionized states,
septet states.

(2)Perturbation selection may be done for doubles.

Restriction

1. Only non-degenerate symmetry is used in this program. For degenerate symmetry, use lower symmetry
   (for example, C2v for linear A-B molecule)

2. Symmetry groups already included are
   C1 Ci, Cs, C2, C2v, C2h, D2, D2h.

Definition

1. KSTATE: state

KSTATE=1 singlet states,
KSTATE=2 triplet states,
KSTATE=3 doublet ionized states,
KSTATE=4 doublet electron-attached (anion) states,
KSTATE=5 quartet ionized states,
KSTATE=7 quintet states,
KSTATE=8 sextet ionized states,
KSTATE=10 septet states.

2. ISYM: space symmetry,

	C_1	C_i	C_s	C_2	C_{2v}	C_{2h}	D_2	D_{2h}
ISYM=1	a	a_g	a'	a	a_1	a_g	a	a_g
ISYM=2		a_u	a''	b	a_2	b_g	b_1	b_{1g}
ISYM=3					b_1	a_u	b_2	b_{2g}
ISYM=4					b_2	b_u	b_3	b_{3g}
ISYM=5								a_u
ISYM=6								b_{1u}
ISYM=7								b_{2u}
ISYM=8								b_{3u}

Perturbation selection

(1) To reduce the number of linked operators within the accuracy you need, perturbation selection is performed for the linked operators. Second-order perturbation energy with the reference state or reference configurations are taken as a criterion for the selection.

(2) HF configuration is utilized as a reference function for the ground state selection. SECI solutions or singly excited configurations chosen as reference configurations from the SECI vectors are utilized for selections of doubly excitation operators for singlet, triplet, doublet ionized, and doublet electron-attached states.

(3) References

H. Nakatsuji, Chem. Phys. 75, 425 (1983).

Input

Namelist Group -- &PRES --

This namelist group is common to both of the SAC-CI SD-*R* part and the SAC-CI general-*R* and high-spin part.

JCALC(ISYM,KSTATE)
JCALC(ISYM,KSTATE)=1: ISYM of KSTATE is calculated. Definition of KSTATE and ISYM is given above.
Default: Transferred from Gaussian)

NOCC
Number of occupied MO's used in integral transformation.
(Default: Transferred from Gaussian)

NVAC
Number of virtual MO's used in integral transformation.
(Default: Transferred from Gaussian)

MSOL(ISYM,KSTATE)
Number of solution for ISYM of KSTATE. Ground state should be included in the number of solution.
(Default: Transferred from Gaussian)

CMAIN(KSTATE)
Threshold of CI coefficient for choosing reference configurations from the SECI vectors.
(Default: CMAIN(KSTATE)=$1.0d^{-1}$)

ISEL(KSTATE)
=0: SECI solutions are used in perturbation selection.
=1: Singly excited configurations and SECI coefficients are used in selection. SECI coefficients are used as weight in perturbation selection.

=2: Singly excited configurations are used in selection. SECI coefficients are not used as weight.
(Default: ISEL(KSTATE)=0)

ESELG
Energy threshold (in au) of perturbation selection for ground state (SAC).
(Default: $1.0d^{-6}$)

ESELE(KSTATE)
Energy threshold (in au) of linked-operator selection for KSTATE of SAC-CI.
(Default: 0.1*ESELG, when ISEL(KSTATE)=0,2. 0.1*ESELG*CMAIN**2, when ISEL(KSTATE)=1.)

Note: Recommended thresholds are
ESELE(KSTATE)=0.1*ESELG for energy calculation,
ESELE(KSTATE)=0.0 for hfsc calculation.

CSPIN(KSTATE)
CSPIN(KSTATE)=1: Impose completeness of spin space for double excitation operators.
(Default: CSPIN(KSTATE)=0)

IPRINT
0 Standard printing
-1 Debug printing
N N = a + b*10 + c*100 + d*1000 + e*10000
a = 1; Equivalent to #P printing
0; None
b = 1; Linked and unlinked operators after the selection
0; None
c = 1; Iterative process
0; None
d = 1; Natural orbitals in MO representation
2; Natural orbitals in AO representation
3; Natural orbitals in both MO and AO representation
0; None
e = 1; Natural orbitals in MO representation
2; Natural orbitals in AO representation
3; Natural orbitals in both MO and AO representation
0; None
(Default: IPRINT=0)

Namelist Group -- &SDPRES --

This namelist group is specific for SAC-CI SD-*R* calculation for
KSTATE = 1 to 4, i.e.
KSTATE=1 singlet states,
KSTATE=2 triplet states,
KSTATE=3 ionized states, and

KSTATE=4 electron-attached (anion) states.
(Corresponding namelist group for SAC-CI general-*R* and high-spin part is given in step #GHPRES#.)

IOCC
Number of occupied MO's in the active space of SAC/SAC-CI
(Default: IOCC = NOCC)

IVAC
Number of virtual MO's in the active space of SAC/SAC-CI
(Default: IVAC = NVAC)

JOCC(KSTATE)
Number of occupied MO's in SECI (reference CI) active space for kstate.
(Default: JOCC(KSTATE)=IOCC)

JVAC(KSTATE)
Number of virtual MO's in SECI (reference CI) active space for kstate.
(Default: JVAC(KSTATE)=IVAC)

MSTATE(ISOL,ISYM,KSTATE), ISOL=1, MSOL(ISYM,KSTATE)
MSTATE(ISOL,ISYM,KSTATE)=1: In perturbation selection for (ISYM,KSTATE), ISOL-th SECI solution for (ISYM,KSTATE) is taken as reference solution. ISOL starts from lowest solution.
(Default: MSTATE(ISOL,ISYM,KSTATE)=1, ISOL=1,MSOL(ISYM,KSTATE))

SEPA(KSTATE)
SEPA(KSTATE)='SEPA': Different energy thresholds are utilized for perturbation selection (for example, for calculations of pi-pi* excited states, better threshold may be used for the pi space than for the sigma space). The excitations within (ISEPMO(i), i=1,NSEPMO) are selected by the energy thresholds ESELG2 and ESELE2. ISEPMO, NSEPMO, ESELG2, and ESELE2 defined below should be given, when SEPA(KSTATE)='SEPA'.
(Default: not 'SEPA')

NSEPMO
Number of ISEPMO.
(NSEPMO should be defined, when SEPA(KSTATE)='SEPA')

ISEPMO(i),i=1,NSEPMO
ISEPMO(i)-th MO belongs to SEPA group. The numbering starts from the lower limit of active space.

ESELG2
Energy threshold (in au) of perturbation selection for a1 ground state(SAC), for SEPA group MOs.

ESELE2(KSTATE)
Energy threshold (in au) of perturbation selection for SAC-CI for SEPA group MOs.

TE

Energy of Hartree-Fock configuration or single determinant (energy standard).
(Default: TE=0.0d0)

Notice for larger scale SAC/SAC-CI calculation

If the number of the selected double excitation operators is larger than the default value of NDOUBLE=100000, give "NDOUBLE" a larger number.

NDOUBLE

Maximum number of double excitation operators after perturbation selection.
(Default: NDOUBLE=100000)

In #sdpres#, the program needs two large arrays. One is for MOERI and the other for workspace to sum up integrals (between linked terms). The program automatically determine MAXERI and MAXCONF with available memory as a standard. You can also control MAXERI and MAXCONF by yourself.

MAXERI

Maximum number of MO 2-electron integrals loaded on memory.
(Default: Optimal parameter is set.)

MAXCONF

Number of configurations taken into perturbation selection routine.
(Default: Optimal parameter is set.)

Sample input

```
&PRES    JCALC(1,1)=1, JCALC(2,1)=1, JCALC(3,1)=1, JCALC(4,1)=1,
         JCALC(1,2)=1, JCALC(2,2)=1, JCALC(3,2)=1, JCALC(4,2)=1,
         JCALC(1,3)=1, JCALC(2,3)=1, JCALC(3,3)=1, JCALC(4,3)=1,
         JCALC(1,4)=1, JCALC(2,4)=1, JCALC(3,4)=1, JCALC(4,4)=1,
         NBF=10, NOCC=4, NVAC=6,
         MSOL(1,1)=2, MSOL(2,1)=1, MSOL(3,1)=1, MSOL(4,1)=1,
         MSOL(1,2)=1, MSOL(2,2)=1, MSOL(3,2)=1, MSOL(4,2)=1,
         MSOL(1,3)=1, MSOL(2,3)=1, MSOL(3,3)=1, MSOL(4,3)=1,
         MSOL(1,4)=1, MSOL(2,4)=1, MSOL(3,4)=1, MSOL(4,4)=1,
         CMAIN(1)=1D-1, CMAIN(2)=1D-1, CMAIN(3)=1D-1, CMAIN(4)=1D-1,
         ISEL(1)=0, ISEL(2)=0, ISEL(3)=0, ISEL(4)=0,
         ESELG=1D-5
         ESELE(1)=1D-6, ESELE(2)=1D-6, ESELE(3)=1D-6, ESELE(4)=1D-6,
         CSPIN=0,0,0,0,0,0,0,0,0,0,
         IPRINT=1, /

&SDPRES IOCC(1)=5, IVAC(1)=6, IOCC(2)=5, IVAC(2)=6,
         IOCC(3)=5, IVAC(3)=6, IOCC(4)=5, IVAC(4)=6,
         JOCC(1)=5, JVAC(1)=6, JOCC(2)=5, JVAC(2)=6,
         JOCC(3)=5, JVAC(3)=6, JOCC(4)=5, JVAC(4)=6,
```

```
MSTATE(1,1,1)=1, MSTATE(1,2,1)=1,
MSTATE(1,3,1)=1, MSTATE(1,4,1)=1,
MSTATE(1,1,2)=1, MSTATE(1,2,2)=1,
MSTATE(1,3,2)=1, MSTATE(1,4,2)=1,
MSTATE(1,1,3)=1, MSTATE(1,2,3)=1,
MSTATE(1,3,3)=1, MSTATE(1,4,3)=1,
MSTATE(1,1,4)=1, MSTATE(1,2,4)=1,
MSTATE(1,3,4)=1, MSTATE(1,4,4)=1,
SEPA(1)='SEPA', SEPA(2)='SEPA',
SEPA(3)='SEPA', SEPA(4)='SEPA',
NSEPMO=4,
ISEPMO(1)=4, ISEPMO(2)=5, ISEPMO(3)=6, ISEPMO(4)=7,
ESELG2=1D-5,
ESELE2(1)=1D-6, ESELE2(2)=1D-6,
ESELE2(3)=1D-6, ESELE2(4)=1D-6,
TE=0D0,
NDOUBLE=100000, /
```

INPUT(I), OUTPUT(0), WORK(W) file information

ifscmo(I), ifscer(I), ifscfi(I), ifscsi(I), ifscsy(O),
ifsccm(O), ifscka(O), ifsch1(O), ifscs1(O), ifscit(O),
ifsciw(W), ifsck1(W)
AGSUM: ifsccg(I), ifscgk(I)

##

---

* Step ci matrix * #CIMX#

In this step, we calculate SD-CI matrix H(i,j) and S(i,j) for each symmetry of
singlet state (KSTATE=1),
triplet state (KSTATE=2),
ionized state (KSTATE=3), and
electron-attached (anionized) state (KSTATE=4).

Input

Namelist Group -- &CIMX --

IPRINT: Level of printing, see &PRES for details.
(Default: IPRINT=0)

Sample input

```
&CIMX IPRINT=-1, /
```

INPUT(I), OUTPUT(0), WORK(W) file information

ifsccm(I), ifscmo(I), ifscer(I), ifscfi(I), ifscsi(I), ifscsy(I),
ifscka(I), ifsck1(I), ifsch1(I), ifscs1(I),
ifschh(O), ifscss(O)
AGSUM: ifsccg(I), ifscgk(I)

##

---

* Step cid * #CID#

Step for iterative diagonalization of CI matrix using Davidson's procedure

---

Namelist Group -- &CID --

EPSQ : Density convergence criterion.
(Default: 1.0d-4)

MIT : Maximum number of iteration per solution.
(Default: 35)

IONLYG: Diagonalize only ground state. This is useful for SAC-CI calculation without TERM3 in step #ULINT#.
0 ... No.
1 ... Yes.
(Default: 0)

MIT2 : Maximum number of iteration per solution for excited state in case of IONLYG=1.
(Default: 2)

IREIT : Reorder initial vectors in increasing energy.
0 ... No.
1 ... Yes.
(Default: 0)

BGSM : 'BGSM' ... Calculate only ground state.
' ' ... Calculate all the states.
(Default: ' ')

IPROC : Print out each iterative process.
0 ... No.
1 ... Yes.

(Default: 0)

FPR : Threshold for printing CI coefficients.
(Default: $1.0d^{-2}$)

IPRINT: Level of printing, see &PRES for details.
(Default: 0)

Sample input

&CID EPSQ=1.D-5, MIT=35, IREIT=0, IPRINT=0, IPROC=0, FPR=1.D-2, /

INPUT(I), OUTPUT(O), WORK(W) file information

ifsccm(I), ifscsi(I), ifschh(I), ifscss(I), ifscit(I),
ifscka(I), ifscrc(O)
AGSUM: ifsccg(I), ifscgk(I)

##

---

* Step ulint * #ULINT#

Step for unlinked integrals for SAC/SAC-CI SD-*R*

#ULINTG#	singlet ground	(SAC)
#ULINTS#	singlet excited	(SAC-CI)
#ULINTT#	triplet	(SAC-CI)
#ULINTIA#	ionized,anionized	(SAC-CI)

For SAC, integrals for the unlinked terms, S(1)*S(1), S(1)*S(2), S(2)*S(2), S(1)*S(1)*S(1), S(1)*S(1)*S(2), and S(1)*S(1)*S(1)*S(1) are evaluated (ULINTG).

For SAC-CI, integrals for R(1)*S(1), R(1)*S(2), R(2)*S(2), R(2)*S(1), R(2)*S(2), R(1)*S(1)*S(1), R(2)*S(1)*S(1), R(1)*S(2)*S(1), and R(1)*S(1)*S(1)*S(1) are evaluated (ULINTS, ULINTT, ULINTIA).
Integrals for R(0)*exp(S), where R(0) means identity operator, are also evaluated in ULINTS.

** Notation **
S(1) : SAC Single Excitation Operator
S(2) : SAC Double Excitation Operator
S(I) : S(1) + S(2)
R(1) : SAC-CI Single Excitation Operator

R(2) : SAC-CI Double Excitation Operator
R(I) : R(0) + R(1) + R(2)
See for details,
H. Nakatsuji, Chem. Phys. Letters, 67, 329,334 (1979).

Namelist Group -- &ULINT --

This namelist group gives the information to evaluate the unlinked integrals.
This namelist group is not required if there are no special requests.
The namelist items and their meanings are as follows.

TERM1 = 'ON ' Unlinked terms <S(I)|H|S(1)*S(1)> (SAC) and <R(I)|H|R(1)*S(1)> (SAC-CI) are added.
TERM2 = 'ON ' Unlinked terms <S(I)|H|S(1)*S(2)> (SAC) and <R(I)|H|R(2)*S(1)> (SAC-CI) are added.
TERM3 = 'ON ' Unlinked terms <S(1)|H|S(1)*S(1)*S(1)> (SAC) and <R(I)|H|R(2)*S(2)> (SAC-CI) are added.
TERM4 = 'ON ' Other higher unlinked terms are added.
(For default values, see tables below.)

** Note **
If SD-INITIAL option is not used in &CNTL, TERM2, TERM3, and TERM4 are forced to be 'OFF' in the SAC-CI.

When TERM4 is activated, complete SAC/SAC-CI is presumed. Namely, all the thresholds for selection should be zero:
(1) eselg and esele should be set to zero in &PRES.
(2) cmaxg, cmaxes, cmaxed, and cmax in &ULINT are automatically set to zero. TERM1 to TERM3 are automatically set to 'ON '. All the unlinked terms are calculated, therefore, overlap integrals are non-symmetric.

TERM4 is active when electron repulsion integrals are allocated in core memory without separation.

Table. Options and Evaluated Unlinked integrals for SAC

	options to activate				
integral type	TERM1	TERM2	TERM3	TERM4	Default
< 0 |H|S(1)*S(1)>	ON/OFF	---	---	---	not-calc.
<S(1)|H|S(1)*S(1)>	ON/OFF	---	---	---	not-calc.
<S(2)|H|S(1)*S(1)>	ON/OFF	---	---	---	not-calc.
<S(1)|H|S(1)*S(2)>	---	ON/OFF	---	---	not-calc.
<S(2)|H|S(1)*S(2)>	---	ON/OFF	---	---	not-calc.
<S(2)|H|S(2)*S(2)>	---	---	---	---	calc.(always)
<S(1)|H|S(1)*S(1)*S(1)>	---	---	ON/OFF	---	not-calc.
<S(2)|H|S(1)*S(1)*S(1)>	---	---	---	ON/OFF	not-calc.
<S(2)|H|S(1)*S(1)*S(2)>	---	---	---	ON/OFF	not-calc.
<S(2)|H|S(1)*S(1)*S(1)*S(1)>	---	---	---	ON/OFF	not-calc.

CMAXG : Threshold for selection of S operators in SAC.
If a S coefficient is larger than CMAXG, it is included in the S(I)*S(I) terms.
The S coefficients for selection are obtained from the CISD result file.
(Default: CMAXG=0.005)

CMAX : Threshold for selection of S(I) operators of SAC, which is used in SAC-CI.
If a S(I) coefficient is larger than CMAX, it is included in the R(I)*S(I) terms.
The S(I) coefficients for selection are obtained from the SAC result file.
(Default: CMAX=0.001)

CMAXES : Threshold for selection of R(1) operators in SAC-CI.
If a R(1) coefficient is larger than CMAXES, it is included in the R(1)*S(I) terms. The R(1) coefficients for selection are obtained
from the CISD result file.
(Default: CMAXES=0.05)

CMAXED : Threshold for selection of R(2) operators in SAC-CI. If a R(2) coefficient is larger than CMAXED, it is included in the R(2)*S(I) terms. The R(2) coefficients for

Table. Options and Evaluated Unlinked integrals for SAC-CI

	options to activate				
integral type	TERM1	TERM2	TERM3	TERM4	Default
<R(1)|H|R(1)*S(1)>	ON-OFF	---	---	---	not-calc.
<R(2)|H|R(1)*S(1)>	ON-OFF	---	---	---	not-calc.
<R(1)|H|R(1)*S(2)>	---	---	---	---	calc.(always)
<R(2)|H|R(1)*S(2)>	---	---	---	---	calc.(always)
<R(1)|H|R(2)*S(1)>	---	ON/OFF	---	---	not-calc.
<R(2)|H|R(2)*S(1)>	---	ON/OFF	---	---	not-calc.
<R(2)|H|R(2)*S(2)>	---	---	ON/OFF	---	calc.(always)
<R(1)|H|R(1)*S(1)*S(1)>	---	---	---	ON/OFF	not-calc.
<R(2)|H|R(1)*S(1)*S(1)>	---	---	---	ON/OFF	not-calc.
<R(2)|H|R(2)*S(1)*S(1)>	---	---	---	ON/OFF	not-calc.
<R(2)|H|R(1)*S(2)*S(1)>	---	---	---	ON/OFF	not-calc.
<S(2)|H|R(1)*S(1)*S(1)*S(1)>	---	---	---	ON/OFF	not-calc.
<R(1)|H|exp(S)>	---	---	---	ON/OFF	not-calc.
<R(2)|H|exp(S)>	---	---	---	ON/OFF	not-calc.
< 0 |H|R(1)S(1)>	---	---	---	ON/OFF	not-calc.

selection are obtained from the CISD result file.
(Default: CMAXED=0.05)

NMOR =/ 0 : Save the space of (ij/kl) by omitting last (NBF-NMOR) MO's which are not used in calculations
= 0 : NMOR = NBF (Default)

NONHF = 'NONHF' : Means that the molecular orbitals used are not canonical MOs determined by the closed-shell Hartree-Fock SCF method. For examples, open-shell RHF, MCSCF, LMO, etc.
= Others : Means that the closed-shell HF SCF orbitals (Default) are used for the reference orbital set.

IPRINT : Level of printing, see &PRES for details.
(Default: 0)

Following parameters are required when TERM2, TERM3, and/or TERM4 are 'ON' and SD-INITIAL is specified in &CNTL.

ISOL1, ISOL2 : Range of CI solutions to search R(2) which has a larger coefficient than CMAXED
If ISOL1=ISOL2=0, then automatically ISOL1=1 and ISOL2=MSOL (Default).

ISOL3 : Search R(2) in ISOL2 - ISOL3-th vectors which have larger coefficient than CMAXED2, and therefore ISOL1 < ISOL2 < ISOL3.If ISOL3=999, this function is ignored (Default).

CMXED2 : Threshold for selection of R(2). See ISOL3 for usage
(Default: 0.01)

Sample Input 1

```
&ULINT    CMAXG=0.001, CMAX=0.001, CMAXES=0.05, CMAXED=0.05,
          TERM1='OFF', TERM2='OFF', NMOR=0, NONHF='HFSCF', IPRINT=0, /
```

Sample Input 2

```
&ULINT    CMAXG=0.001, CMAX=0.001, CMAXES=0.05, CMAXED=0.05,
          TERM1='ON ', TERM2='ON ', TERM3='ON ',
          NMOR=0, NONHF='HFSCF', IPRINT=0,
          ISOL1=0, ISOL2=0, ISOL3=0, CMXED2=0.05, /
```

Since this sample requires the CISD coefficients to select R(2), SD-INITIAL option must be used in &CNTL.

INPUT(I), OUTPUT(0), WORK(W) file information

ifsccm(I), ifscmo(I), ifscer(I), ifscfi(I), ifscsi(I), ifscsy(I),
ifscka(I),
ifsh24(O), ifsh02(O), ifsckx(O), ifscun(O), ifwhfs(O)
AGSUM: ifsccg(I), ifscgk(I), ifscul(I), ifscgr(I)

```
################################################################################

* Step saceq *                                   #SAC#

                    Step for iterative solution of the SAC equation (SAC-NV)

--------------------------------------------------------------------------------

  Input

    Namelist Group -- &SAC --

      IPRINT : Level of output, See &PRES for details.
               (Default: 0)

  Technical parameters for SAC calculation
==========================================================================
    Following variables control the methods and conditions in the SAC calculation.
    You need not input them because the default values are good in most cases.

      IDIIS : Select the convergence method to solve SAC equation.
              = 0 : Use DIIS. (Default)
              = 1 : Not use DIIS.
      -- About DIIS see--
        P. Pulay, Chem. Phys. Letters, 73, 393 (1980).

      IRESTT : If the calculation is interrupted before convergence, you can restart from the vectors
                stored in file.
                (Default = 1 in RESTART job. See guide for &CNTL. = 0 otherwise. )
                = 0 :    Normal.
                =/ 0 :    Initial vector is read from file.

      MAXSAC : Maximum number of iteration for SAC equation.
                (Default: 20)

      EPSSAC : Threshold for convergence of SAC equation.
               (Default: 1.0d-7)

      MAXLIN : Maximum number of iteration for linear equation.
                (Default: 200)

      EPSLIN : Threshold for convergence of linear equation.
               (Default: 1.0d-7)

      OMEGA    : If IDIIS=0,
                 experimental cut-off parameter.
                 (Default: 0.01)
                 If IDIIS=1, damping factor in linear equation. (make smaller as molecules become
```

larger.)

(Default: 0.79)

==========

Sample input 1 (with DIIS)

```
&SAC IPRINT=0, IDIIS=0, IRESTT=0,
        MAXSAC=20, EPSSAC=1.0d-7, MAXLIN=99, EPSLIN=1.0d-7,
        OMEGA=0.01, /
```

Sample input 2 (without DIIS)

```
&SAC IPRINT=0, IDIIS=1, IRESTT=0,
        MAXSAC=20, EPSSAC=1.0d-7, MAXLIN=99, EPSLIN=1.0d-7,
        OMEGA=0.79, /
```

INPUT(I), OUTPUT(O), WORK(W) file information

ifsccm(I), ifscsi(I), ifscka(I), ifscgk(I), ifschh(I), ifscss(I),
ifscit(I), ifsh24(I), ifsh02(I), ifscka(I),
ifscsv(O), ifscsn(O)
AGSUM: ifsccg(I), ifscgk(I)

##########

---

* Step dsaceq * #DSAC#

Step for solution of SAC equation by direct solution of linear equation (SAC-NV)

Namelist group -- &DSAC --

IPRINT : Same as in step #SAC#.

Technical parameters for SAC direct calculation

==========

Following variables control the methods and conditions used in SAC direct calculation.
You need not input them because the default values are good in most cases.

IRESTT, MAXSAC, EPSSAC : Same as in step #SAC#.

IDAMP : Control of damping factor.
=1 : Set dumping factor. (Default)
=0 : Do not set damping factor.

FDAMP : Dumping factor multiplied to the unlinked term. Physically, this factor should finally become 1.0.
(Default: 1.0)

==========

Sample input

```
&DSAC    IPRINT=0,
         IRESTT=0, MAXSAC=20, EPSSAC=1.0d-7, IDAMP=1, FDAMP=1.0, /
```

INPUT(I), OUTPUT(O), WORK(W) file information

File I/O in step #DSAC# is same as in step #SAC#

##

---

* Step dsciv * #SCIV#

Step for diagonalization of SAC-CI-V(variational) matrix by iterative procedure

You can include |0> within variable space and solve SAC-CI vectors including (pseudo)-SAC wf. in the solution space.

Input

Namelist Group -- &SCIV --

IN2ND : Whether second-order terms are included or not.
See ** Remarks ** below
0 ... Not include second-order terms (script-S).
2 ... Include only script-S and consider orthogonality between ground and excited states.
(Default: 0)

** Note **
Except for singlet A1 excited state, this option is not used. When SAC-CI gradients are selected, script-S-part is not included.

INHFC : Include Hartree-Fock configuration |0> within variable space.
0 ... No
1 ... Yes
(Default: 1)

EPSQ : Density convergence criterion

(Default: $1.0d^{-5}$)

MIT : Maximum number of iteration per solution
(Default: 35)

IPROC : Print out iterative procedure
0 ... No
1 ... Yes
(Default: 0)

FPR : Threshold for printing out SAC-CI coefficients
(Default: $1.0d^{-1}$)

IPRINT : Level of printing, see &PRES for details.
(Default: IPRINT=0)

** Remarks for steps #SCIV#, #DAS#, #SCINV# and #DNAS# **

Method
1. Not include second-order terms
Not include |0> within variable space (recommended for SAC-CI-NV calculation)
2. Include |0> within variable space and consider orthogonality between 'ground' and excited states
'ground' means the pseudo-SAC wf in the same space (Recommended)
3. Include only script-S part (recommended for SAC-CI-V calculation)

** Note **
(1) The meaning of script-S is different between the SAC-CI-V and SAC-CI-NV methods, so that recommended calculations are different.
(See for details, H. Nakatsuji, Chem. Phys. Lett. 67, 337 (1979).)

Table. Correspondence of parameters among SAC-CI diagonalization programs

Method	Step						
	#SCIV#		#SCINV#		#DAS# and #DNAS#		
Type	IN2ND	INHFC	INHFC	ISCRPT	WITHHF	KSYM	SCRPTS
1	0	0	0	0	'SAC-CI'	9	' '
2	0	1	1	0	'WITHHF'	9	' '
3	2	0	0	1	'SAC-CI'	9	'SCRPTS'

(2) In high-spin and general-*R* calculations, istep controls the function of "SCIV".
istep = 2 : single and double CI
= 4 : reference EGCI
= 5 : EGCI
= 6 : SAC-CI-V general-*R*

Sample input

&SCIV IN2ND=2, INHFC=0, EPSQ=1.D-5, MIT=35, IPRINT=0, /

INPUT(I), OUTPUT(O), WORK(W) file information
SD-*R*
ifsccm(I), ifscsi(I), ifscka(I), ifschh(I), ifscss(I), ifscit(I),
ifscun(I),
ifscsv(O)
AGSUM: ifsccg(I), ifscgk(I)

high-spin and general-*R*
ifcom(I)

##

---

* Step Diags * #DAS#

Step for InCoreDirect(D) diagonalization of symmetric matrix(A) with overlap(S) for CI and SAC-CI-V

Istep	Excitation operators	Hamiltonian matrix	Overlap matrix	Unlinked integrals	Solutions
2	iflabb(I)	ifhmx2(I)	ifsmx2(I)	---	ifsol2(O)
4	iflbre(I)	ifhmre(I)	ifsmre(I)	---	ifslre(O)
5,6	iflabe(I)	ifhmx3(I)	ifsmx3(I)	ifumx3(I)	ifsol3(O)

Input

Namelist Group -- &DAS --

METHOD : Type of calculation.
' CID' ... direct diagonalization for #CID#.
' SCIV' ... direct diagonalization for #SCIV#.
(Default: Controlled by &CNTL)

JSOL(I,J) : Number of solutions for I-isym and J-kstate in this diagonalization step.
For example, JSOL(2,1)=3 means 3 solutions for 2nd symmetry of singlet state
(Default: JSOL(I,J)=MSOL(I,J))

WITHHF : This option is only for singlet A1 excited states.
If WITHHF='WITHHF', Hartree-Fock (reference) configuration is included for both KSYM=1 (ground state) and KSYM=9 (singlet excited state). Dimensions are as follows.
N=Nds+Ndd+1 for WITHHF='WITHHF', and
N=Nds+Ndd for WITHHF='SAC-CI'.
(Default: 'WITHHF' for CI and 'WITHHF' for SAC-CI)

SCRPTS : "script-S-part" is done as follows.
'SCRPTS' ... include script-S-part
others ... not include script-S-part (Default).

** Note **

Except for singlet A1 excited state, this option is not used. When SAC-CI gradients are selected, script-S-part is not included.

Istep	Excitation operators	Hamiltonian matrix	Overlap matrix	Unlinked integrals	Solutions
1	iflabr(I)	ifhmx1(I)	ifsmx1(I)	---	ifsol1(O)
2	iflabb(I)	ifhmx2(I)	ifsmx2(I)	---	ifsol2(O)
4	iflbre(I)	ifhmre(I)	ifsmre(I)	---	ifslre(O)
5,6	iflabe(I)	ifhmx3(I)	ifsmx3(I)	ifumx3(I)	ifsol3(O)

FPR : Threshold for printing out SAC-CI coefficients.
(Default: 1.0d-1)

IPRINT : Level of printing, see &PRES for details.
(Default: 0)

** Note **

In SAC-CI-V calculation, recommended choice is WITHHF='WITHHF', (KSYM=9,) and SCRPTS=' '.

See ** Remarks ** in #SCIV#

In high-spin and general-*R* calculations, ISTEP controls the function of "DAS".

ISTEP= 1 : reference-CI
= 2 : single and double CI
= 4 : reference-EGCI
= 5 : EGCI
= 6 : SAC-CI-V general-*R*

Sample input

&DAS JSOL(2,1)=3, IPRINT=0, /

INPUT(I), OUTPUT(O), WORK(W) file information

SD-*R*

File I/O in step #DAS# is same as in step #SCIV# for SAC-CI-V or in step #CID# for CI.

high-spin and general-*R*

---

* Step Dscinv * #SCINV#

Step for diagonalization of SAC-CI-NV(non-variational) matrix (non-symmetric) by iterative procedure

The method is described in
K. Hirao and H. Nakatsuji, J. Comp. Phys. 45, 246 (1982).

You can include |0> within variable space and solve SAC-CI vectors including pseudo-SAC wf. in the solution space.

See ** Remarks ** in #SCIV#

Namelist Group -- &SCINV --

INHFC : Include Hartree-Fock configuration |0> within variable space.
0 ... No
1 ... Yes
(Note : This option corresponds to WITHHF of DNAS, etc.)
(Default: 1)

ISCRPT : Include script-S part.
0 ... No
1 ... Yes
** Note **
Except for singlet A1 excited state, this option is not used. When SAC-CI gradients are selected, script-S-part is not included.
(Default: 0)

EPSQ : Density convergence criterion
(Default: $1.0d^{-4}$)

MIT : Maximum number of iteration per solution
(Default: 35)

IPROC : Print out iterative procedure
0 ... No
1 ... Yes
(Default: 0)

FPR : Threshold for printing out SAC-CI coefficients
(Default: 1.0d-1)

IPRINT: Level of printing, see &PRES for details.
(Default: 0)

Sample input

&SCINV INHFC=0, ISCRPT=0, EPSQ=1.D-5, MIT=35, IPRINT=0, /

INPUT(I), OUTPUT(O), WORK(W) file information
SD-*R*
ifsccm(I), ifscsi(I), ifscka(I), ifschh(I), ifscss(I), ifscit(I),
ifscun(I),
ifscsn(O)
AGSUM: ifsccg(I), ifscgk(I)

high-spin and general-*R*
ifcom(I), iflabe(I), ifhmx3(I), ifsmx3(I), ifumx3(I), ifsl3n(O)

##

---

* Step Diagnas * #DNAS#

Step for InCoreDirect diagonalization of non-symmetric SAC-CI-NV matrix with overlap

---

Input

Namelist Group -- &DNAS --

JSOL(I,J): Number of solutions for I-isym and J-kstate in this diagonalization step.
For example, JSOL(2,1)=3 means 3 solutions for 2nd symmetry of singlet state
(Default: JSOL(I,J)=MSOL(I,J))

WITHHF : This option is only for singlet A1 excited states.
If WITHHF='WITHHF', Hartree-Fock (reference) configuration is included for both KSYM=1(ground state) and
KSYM=9(singlet excited state) calculations.
Dimensions are as follows.
N=Nds+Ndd+1 for WITHHF='WITHHF', and
N=Nds+Ndd for WITHHF='SAC-CI'.
(Default: 'WITHHF')

SCRPTS : "script-S-part" is done as follows.
'SCRPTS' ... include script-S-part
others ... not include script-S-part (Default).
(Gradient calculation is adapted to this case.)
** Note **
Except for singlet A1 excited state, this option is not used.
When SAC-CI gradients is selected, script-S-part is not included.

FPR : Threshold for printing out SAC-CI coefficients.
(Default: $1.0d^{-1}$)

IPRINT : Level of printing, see &PRES for details.
(Default: 0)

** Note **
In SAC-CI-NV calculation, recommended choice is WITHHF='WITHHF' and SCRPTS=' '.
See ** Remarks ** in #SCIV#

Sample input

&DNAS JSOL(2,1)=3, IPRINT=0, /

INPUT(I), OUTPUT(O), WORK(W) file information

File I/O in step #DNAS# is same as in Step #SCINV#

##

---

* Step DENSITY* #DENS#

Step for density matrix, natural orbitals, transition density matrix, and spin density matrix

See,
H. Nakatsuji and K. Hirao, Int. J. Quantum Chem. 20, 1301 (1981)

Input

Namelist Group -- &DENS --

This step calculates density, transition density, and spin-density matrices. Type of calculation is controlled by step #SUPER97#.

If the following subkeywords were specified in &CNTL, SINGLET, TRIPLET, etc., the corresponding calculation will be done in this step.
(See input &CNTL of step #SUPER97#.)

Scheme. Job of #DENS#

&CNTL	Output of step #DENS#
PROPERTY	Density matrices and natural orbitals of all the states

TRANS Transition density matrices between the lowest state and all other states

HFSC Spin density matrices of all the states

For singlet state, transition density between SAC state and SAC-CI states or between SAC-CI states are calculated. For other spin-symmetries, transition density between SAC-CI states are calculated. In such case, state which is the lowest in energy is selected as the "ground state" automatically.

CMAX : Threshold for the coefficient of S(2) operator included in the unlinked terms of SAC-CI.
(Default: $1.d^{-3}$)

CR1MAX : Threshold for the coefficient of R(1) operator included in the unlinked terms of SAC-CI.
(Default: $1.d^{-1}$)

ISSCIG
=0 : Ground state is SAC when calculating transition density
=1 : Ground state is SAC-CI state and is specified by KSTATT,ISYMTT,ISOLTT.
(Default: Automatically determined using SAC/SAC-CI energies.)

KSTATT,ISYMTT,ISOLTT:
Transition density between the ISOLTT-th state of ISYMTT symmetry and other states for KSTATT spin state.
(ISOLTT should be counted without ground-state SAC)
(Default: SAC-CI state of lowest energy is automatically selected.)

ILEFT
=0 : Only right vectors are used.
=1 : Left vectors and right vectors are used.
See Sec. I-E for details.
(Default: 0)

WITHHF='WITHHF' : Hartree-Fock is included in SAC-CI singlet state.
See step #SCIV# for details.
(Default: 'WITHHF')

SCRPTS='SCRPTS' : Orthogonality between SAC and SAC-CI states is considered in SAC-CI singlet state. This option cannot be used with WITHHF='WITHHF'. See step #SCIV# for details.
(Default: ' ')

Information of WITHHF and SCRPTS are transferred from diagonalization steps (SCIV, SCINV, DAS, DNAS).

ICALHI : Calculation of higher-order unlinked terms R(2)*S(2) in SAC-CI.
=0 : No

=1 : Yes
(Default: 0)

THRECCC : Threshold for calculating density and transition density matrix in the unlinked terms
(Default: $1.d^{-5}$)

IPRINT : Level of printing, see &PRES for details.
(Default: 0)

Note
The unlinked terms evaluated in this step are R(1)*S(2) and R(2)*S(2). Others are not implemented.

Sample input

```
&DENS CMAX=1.d-3, CR1MAX=1.d-1, ILEFT=1, WITHHF='WITHHF',
      SCRPTS='SSSSSS', IPRINT=0, /
```

INPUT(I), OUTPUT(0), WORK(W) file information

ifsccm(I), ifscsi(I), ifscka(I),
ifscsv(I: SAC-CI-V), ifscsn(I: SAC-CI-NV),
ifscno(O: Property), ifsctd(O: Tran or Hfsc)
AGSUM: ifsccg(I), ifscgk(I)

##

---

* Step property * #PROP#

In this step, one-electron properties are calculated as follows:

1. one-electron properties using SAC/SAC-CI density
2. transition properties using SAC-CI transition density
3. hyperfine splitting constants using SAC-CI spin density
4. population analysis of SAC/SAC-CI.

For Gaussian version, NAMELIST input is not available; only KEYWORD input is available.

Properties are calculated as the expectation values of the property-operators for the SAC/SAC-CI densities calculated instep #DENS#. Property operator integrals are evaluated with PRISM algorism (Subroutine 'OneElI').
See Programmer's Reference for details.

KEYWORDS

*Calculate multipole moment
'NoMultipole' not calculate multipole moment
'Dipole' calculate monopole and dipole moment (default)
'Quadrupole' calculate monopole, dipole and quadrupole moment
'Octapole' calculate monopole, dipole, quadrupole and octapole moment
'Hexadecapole' calculate monopole, dipole, quadrupole, octapole and hexadecapole moment

*Calculate electrostatic properties
'NoES' not calculate electrostatic properties (default)
'ESPotential' calculate electric potential
'ESField' calculate electric potential and electric field
'ESFieldGradient' calculate electric potential, electric field and electric field gradient

*Calculate n-th moment
'NoMoment' not calculate n-th moment
'SecondMoment' calculate second moment (default)
'ThirdMoment' calculate second and third moment
'FourthMoment' calculate second, third and fourth moment

*Calculate diamagnetic properties
'NoDiamagnetic' not calculate diamagnetic properties (default)
'Shielding' calculate diamagnetic shielding
'Susceptibility' calculate diamagnetic susceptibility
'ShieldSuscept' calculate diamagnetic shielding and susceptibility

---

INPUT(I), OUTPUT(0), WORK(W) file information

ifscno(I), ifsctd(I)

##

II-B. SAC and SAC-CI SD-*R* Part (Sub steps) (See Table 2 of Part I-D-1)

##

* Step fock * #FOCK#

Step to calculate fock matrix for non-canonical MO's.

When non-canonical MO's have been used in SCF step, this step is called from #BPRES#.
For molecules having odd number of electrons, this program adds one electron to make closed shell in the default procedure. When keyword "SubElectron" is specified, this program remove one electron to make closed shell one.

REMARK
User's Reference : spin multiplicity, electric charge, RO prefix.

MyIOp(237) =0 : Use canonical MOs (closed-shell RHF).
=1 : Use non-canonical MOs. (ROHF, CASSCF).

##

---

* Step gsum * #GSUM#

This step forms a common set (group sum = GSUM) of excitation operators selected at several geometries 1,2,...,N.
This step is necessary for calculations using perturbation selection scheme for

1. Potential energy curves
   Smooth potential energy curve is guaranteed.

2. Energy gradients
   In the energy gradient calculations using perturbation selection, GSUM method is used. GSUM provides a common set of excitation operators for all the geometries, and removes the problem of discontinuity of the energy gradients. Consequently, smooth convergence is obtained in the SAC/SAC-CI energy gradients.

In this step, we prepare
(1) group-sum of linked S and R operators
(2) group-sum of S(i)-operators to be used in the unlinked terms of SAC and SAC-CI calculations.
(3) group-sum of R(1) and R(2)-operators to be used in the unlinked terms of SAC-CI calculations.

Notes:
(1) Select geometries in the region of geometrical parameters.
(2) The MO's at different geometries are arranged in the same order in nature as the standard one in L511 and saved at 524 in RW file.
(3) For more detail, see
H. Nakatsuji, J. Ushio, and T. Yonezawa, Can. J. Chem. 63 1857 (1985).
T. Nakajima and H. Nakatsuji, Chem. Phys. Lett. 280, 79 (1997), Chem. Phys. 242, 177 (1999).
(4) GSUM is performed by Multi-Step jobs for potential energy calculation. (see Job stream I)
(5) GSUM is performed automatically in geometry optimization calculation. (see Job stream II)
(6) GSUM is available only for SAC/SAC-CI SD-*R* calculations of singlet, triplet, ionized, and electron attached states.

Job stream I: potential energy curve
Gsum at geometries (1,2,...,N) for SAC/SAC-CI calculations at geometries (1',2',...,N')
All geometries must be handled using the same symmetry group.

(1) SDCI calculations are carried out and group-sum is performed for excitation operators successively for all the geometries (1,2,...,N). The SAC-CI subkeyword should be specified as 'BGSUM' (Before GSUM) for the first geometry and 'CGSUM' (construct GSUM) for the rest,

i.e.,

```
For geometry  1     BGSUM
For geometry  2     CGSUM
    --------          CGSUM
For geometry N    CGSUM
```

(2) Using the obtained group-summed S and R operators, SAC/SAC-CI calculations are performed under the flag AGSUM (After GSUM) for all the geometries (N',...,2',1'). It is recommended to do the SAC-CI calculations in the reverse order of geometries of (1) to get MO correspondence between N and N'.

```
For geometry N'    AGSUM
          ...
For geometry 2      AGSUM
For geometry 1      AGSUM
```

Notes:

It is possible to choose geometries (1',2',...,N') independently from the reference geometries (1,2,...,N). (Normally N' > N)

Job stream II: geometry optimization

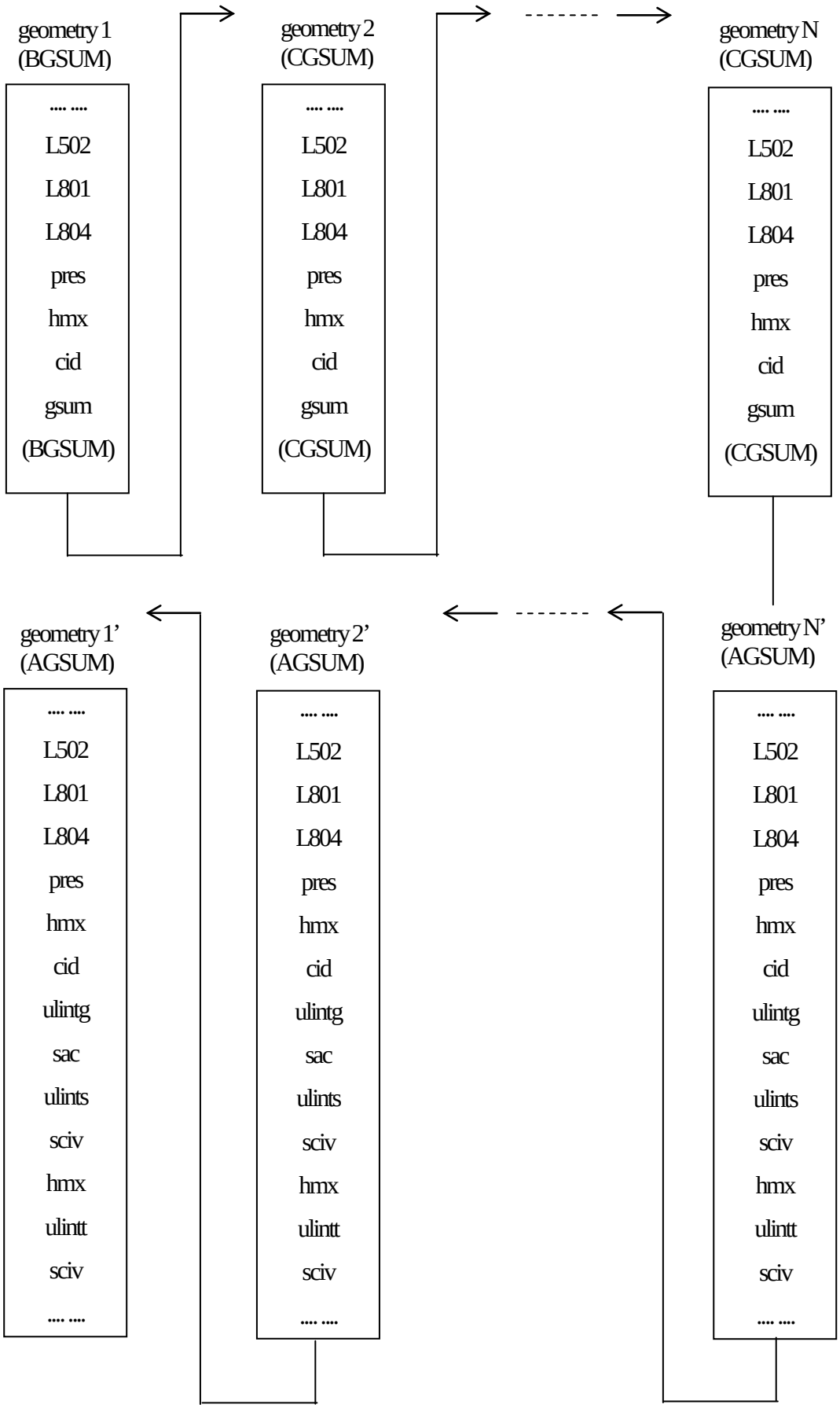
In the cases that important coordinates of potential energy surfaces (PES) is known, geometry optimizations on PESs defined by GSUM method can be carried out simply by adding AGSUM type input with Opt (here denoted by AGSUM + Opt) following BGSUM-(CGSUM)n sequence (the upper part of a figure shown above). To search for stationary points of many PESs by GSUM, i.e., in a common configurational subspace for all the states, repeat (AGSUM + Opt) each TargetRoot following BGSUM-(CGSUM)n sequence. A sample input will be shown.

If the coordinates are unknown (or too many to do GSUM), single-step job including Opt (non-GSUM Opt) is also available. A non-GSUM Opt is equivalent to a BGSUM-(AGSUM + Opt) combination with the same geometry. Notice that &GSUM options are ignored in the non-GSUM case.

See also instructions of SAC/SAC-CI analytical energy gradient part elsewhere.

REMARK

One can obtain optimized geometries of a reactant and a product, for example, of a chemical reaction by this algorithm but can not directly compare their energies because the final set of operators used to optimize them may be different from each other. The GSUM method must be used over the reactant and the product.


geometry 1
(BGSUM)
....
L502
L801
L804
pres
hmx
cid
gsum
(BGSUM)
geometry 2
(CGSUM)
....
L502
L801
L804
pres
hmx
cid
gsum
(CGSUM)
geometry N
(CGSUM)
....
L502
L801
L804
pres
hmx
cid
gsum
(CGSUM)
geometry N'
(AGSUM)
....
L502
L801
L804
pres
hmx
cid
ulintg
sac
ulints
sciv
hmx
ulintt
sciv
....
geometry 2'
(AGSUM)
....
L502
L801
L804
pres
hmx
cid
ulintg
sac
ulints
sciv
hmx
ulintt
sciv
....
geometry 1'
(AGSUM)
....
L502
L801
L804
pres
hmx
cid
ulintg
sac
ulints
sciv
hmx
ulintt
sciv
....

Input

Namelist Group -- &GSUM --

CSMAXG
Threshold for s(i) operators included in the unlinked terms of sac.
(Default: 0.005)

CSMAXE
Threshold for s(i) operators included in the unlinked terms of sac-ci.
(Default: 0.001)

CR1MAX
Threshold for r(1) operators included in the unlinked terms of sac-ci.
(Default: 0.05)

CR2MAX
Threshold for r(2) operators included in the unlinked terms of sac-ci.
(Default: 0.05)

TERM3
Same as &ULINT for SAC-CI
(Default: 'ON ')

ISYSOL(ISYM,KSTATE)
=0 : Group sum is not considered for ISYM and KSTATE.
=1 : Group sum for ISYM.
(Default: ISYSOL(ISYM,KSTATE)=JCALC(ISYM,KSTATE))

NSOL(ISYM,KSTATE)
Number of solution for ISYM,KSTATE.
(Default: NSOL(ISYM,KSTATE)=MSOL(ISYM,KSTATE))

IPRINT: Level of printing, see &PRES for details.
(Default: IPRINT=0)

Sample input

(1) Potential energy curve

```
%Chk=gsum
# SAC-CI(Singlet=Nstate=1 BGSUM)/6-31G

    sample geometry 1

    molecule specification
```

```
--Link1--

%Chk=gsum
# SAC-CI(Singlet=Nstate=1 CGSUM)/6-31G

     sample geometry 2

     molecule specification

--Link1--

%Chk=gsum
# SAC-CI(Singlet=Nstate=1 AGSUM)/6-31G

     geometry 1'

     molecule specification
```

(2) Energy Gradient

```
%Chk=gsum
# SAC-CI(Singlet=Nstate=1 BGSUM)/6-31G

     sample geometry 1

     molecule specification

--Link1--

%Chk=gsum
# SAC-CI(Singlet=Nstate=1 CGSUM)/6-31G

     sample geometry 2

     molecule specification

--Link1--

%Chk=gsum
# SAC-CI(Singlet=Nstate=1 AGSUM)/6-31G Opt

     geometry 1'

     molecule specification
```

INPUT(I), OUTPUT(0), WORK(W) file information

ifsccm(I), ifscsi(I), ifscka(I), ifscit(I),
ifsccg(O), ifscgk(O), ifscul(O), ifscgr(O)

##

---

* Step Satei * #SATEI#

This step calculates monopole intensity of the ionized state.

Input

Namelist Group -- SATEI --

ISOL(ISYM)
Number of solution for ISYM.
(Default: ISOL(ISYM)=MSOL(ISYM,3))

Sample input
&SATEI ISOL=20,10,20,20, /

INPUT(I), OUTPUT(O), WORK(W) file information
SD-*R*
ifsccm(I), ifscsv(I: SAC-CI-V), ifscsn(I: SAC-CI-NV)

general-*R*
ifcom(I), ifsol3(I: SAC-CI-V), ifsl3n(I:SAC-CI-NV),
ifsols(I), iflabe(I), iflabs(I)

##

---

* Step Iopc * #IOPC#

Step to transform IOp input to SAC-CI (Namelist) input. (In case of IOp(99)=1, Namelist input is activated.)

NO INPUT(I), OUTPUT(0) on file

##

---

* Step Fio * #FIO#

File I/O interface to read-write file and check point file.

---

iosccm : I/O of the common information of SAC/SAC-CI
scarrd : defines the file numbers for SAC-CI SD-*R*
scfio2 : saves data with unknown length by successively extending read-write file.

INPUT(I), OUTPUT(0) file information

ifsccm(I/O)

##

---

* Step common change * #COMCG#

Step to rewrite information in the common file

Namelist group -&PRINT-

iprint =0, Print out common file after change except for cien and scien
=1, Print out common file after change
=2, Print out common file before change except for cien and scien, and not alter common file
=3, Print out common file before change, and not alter common file
=4, Print out common file before and after change except for cien and scien
=5, Print out common file before and after change

Namelist group -&CHANGE-

Some variables and arrays defined in #PRES# can be altered in this step.

JCALC(ISYM,KSTATE)
JCALC(ISYM,KSTATE)=1: ISYM of KSTATE is calculated.

MSOL(ISYM,KSTATE)
Number of solution for ISYM of KSTATE.

Sample input

&PRINT IPRINT=5, &END
&CHANGE ICALC(1)=0,ICALC(2)=1, &END

INPUT(I), OUTPUT(0), WORK(W) file information

ifsccm(I/O)

##

II-C. SAC-CI General-*R* and High-Spin Part (See Table 3 of Part I-D-3)

##

---

* Step GHPRES * #GHPRES#

Lower-order excitation operators are generated for
SAC-CI general-*R* and high-spin calculations.

Namelist group &PRES is common between #PRES# for SAC-CI SD-R and #GHPRES#. Namelist group &GHPRES is necessary only for SAC-CI general-*R* and high-spin calculations.

Input
Namelist Group -- &PRES --

JCALC(ISYM,KSTATE), MSOL(ISYM,KSTATE), CMAIN(KSTATE), ISEL(KSTATE), ESELG, ESELE(KSTATE), CSPIN(KSTATE), IPRINT:

These input are common to those given in the Namelist &PRES in step #PRES# except for KSTATE running through KSTATE=1 to KSTATE=10.
(Default: See step #PRES#)

Namelist Group -- &GHPRES --

MAXEXC(KSTATE)
Maximum order of excitations for R-operators
This value is limited up to 6 (sextuples).
(Default: 6(general-*R*)
2(high-spin))

MSOL1(ISYM,KSTATE)
Number of solutions of reference-CI calculations for ISYM and KSTATE. Reference-CI is done in the small active space, see below.
(Default: msol1(isym,kstate)=msol(isym,kstate)
At least 3 for singlet, 1 for all other states,
even if msol(isym,kstate)=0 in general-*R*)

MSOL2(ISYM,KSTATE)
Number of solutions of A-CI or B-CI within the space of singles and doubles (doubles and triples for quartet and quintet, triples and quadruples for sextet and septet) for ISYM of KSTATE. A-CI or B-CI is done in the large active space, see below.
(Default: msol2(isym,kstate)=msol(isym,kstate)
At least 3 for singlet, 1 for all other states,
even if msol(isym,kstate)=0 in general-*R*)

In SAC-CI general-*R* and high-spin calculations, we recommend to use small active space in reference-CI calculation. Since reference-CI is done by InCoreDiag diagonalization (step #DAS#), the computational cost can be reduced using small nocc2 and nvac2. For this purpose, small active space is defined by NOCC2 and NVAC2.

```
|<-------------------- Total active space of SAC/SAC-CI--------------------->|
|<--------------NOCC------------->|<----------------NVAC ---------------->|  : large active
|                                 |                                        space
|          |<-------NOCC2 ----->|<------NVAC2 ------>|                      : small active
|                                 |                                        space
```

NOCC2
Number of occupied MO's in small active space for reference CI
(Default: Automatically determined.)

NVAC2
Number of unoccupied MO's in small active space for reference CI
(Default: Automatically determined.)

** Note **
If NOCC2 and NVAC2 are not given, they are determined automatically using MXDIAG and dimensions of reference-CI. When the large scale reference-CI is necessary, MXDIAG should be increased. See also MXDIAG.

MXDIAG
Maximum dimension of reference-CI
(Default: 2000)

NUNIT
Unit of storing resultant excitation operators temporarily
(Default : 10000)

** Note **
Orders of excitation operator are different between low-spin (singlet to triplet) and high-spin (quartet to septet) states. Namely, terms "singles" and "doubles" should be interpreted

as "doubles" and "triples", respectively, for quartet and quintet states in the following explanations.

IAOP(1-3)

Type of generating A-operators (only for SAC-CI general-*R*)

IAOP(1) : Type of reference-CI

=1 : r(1) (singles)

=2 : r(1),r(2) (singles and doubles)

IAOP(2) : Active space of reference-CI

=1 : Large active space specified by NOCC and NVAC

=2 : Small active space specified by NOCC2 and NVAC2

IAOP(3) : Perturbation selection for SD-CI(A-CI)

=1 : Without perturbation selection

=2 : With perturbation selection

(Default: 2,2,2 only for general-*R*)

** Note **

(1) If singlet excited state is calculated, IBOP is used instead of IAOP for generating A-operators.

(2) Only IBOP is used for SAC-CI high-spin.

IBOP(1-3,KSTATE)

Type of generating B-operators

IBOP(1,KSTATE) : Type of reference-CI

=1 : r(1) (singles)

=2 : r(1),r(2) (singles and doubles)

IBOP(2,KSTATE) : Active space of reference-CI

=1 : Large active space specified by NOCC and NVAC

=2 : Small active space specified by NOCC2 and NVAC2

IBOP(3,KSTATE) : Perturbation selection for SD-CI(B-CI)

=1 : Without perturbation selection

=2 : With perturbation selection

(Default: 2,2,2 for general-*R*)

1,2,2 for high-spin)

NEGREF

Reference-EGCI is performed for determining the reference operators for perturbation selection.

=0: reference-SDCI

=1: reference-EGCI

(Default: 0)

NSELSH

Perturbation selection is performed for doubles(D) for quartet and quintet, triples(T) for sextet and septet in SAC-CI high-spin.

This option is useful for SAC-CI high-spin, where DT is generated in quartet and quintet states.

=0: Do not selection for D(quartet and quintet) or T (sextet and septet)

=1: Do selection for D or T

(Default: 1)

NTGENH

Type of generating higher-order terms

=0: Exponentially-generation scheme is used.

=1: All the higher-order terms up to triples (for singlet and triplet states) or quadruples (for ionized, anionized, quartet states) are generated for selection.

(Default: 0)

ISKIPH

Type of selecting higher-order terms for calculating unlinked integrals in case of NTGENH=1.

=0: small CI is done.

=1: small CI is skipped.

(Default: 0)

Note:

ISTEP controls the function of step #GHPRES#.

istep =1: Generation of excitation operators for reference-CI

=2: Generation of SD-CI(A-CI or B-CI) excitation operators

Sample input

```
&PRES
   JCALC(1,5)=1, JCALC(2,5)=1, JCALC(3,5)=1, JCALC(4,5)=1,
   JCALC(1,7)=1, JCALC(2,7)=1, JCALC(3,7)=1, JCALC(4,7)=1,
   JCALC(1,8)=1, JCALC(2,8)=1, JCALC(3,8)=1, JCALC(4,8)=1,
   JCALC(1,10)=1, JCALC(2,10)=1, JCALC(3,10)=1, JCALC(4,10)=1,
   MSOL(1,5)=1, MSOL(2,5)=1, MSOL(3,5)=1, MSOL(4,5)=1,
   MSOL(1,7)=1, MSOL(2,7)=1, MSOL(3,7)=1, MSOL(4,7)=1,
   MSOL(1,8)=1, MSOL(2,8)=1, MSOL(3,8)=1, MSOL(4,8)=1,
   MSOL(1,10)=1, MSOL(2,10)=1, MSOL(3,10)=1, MSOL(4,10)=1,
   ISEL(5)=2, ISEL(7)=2, ISEL(8)=2, ISEL(10)=2,
   ESELG=1.d-5,
   ESELE(5)=1.d-6, ESELE(7)=1.d-6, ESELE(8)=1.d-6, ESELE(10)=1.d-6,
   CMAIN(5)=0.1, CMAIN(7)=0.1, CMAIN(8)=0.1, CMAIN(10)=0.1,
   CSPIN(5)=1, CSPIN(7)=1, CSPIN(8)=1, CSPIN(10)=1,
/
&GHPRES
   MAXEXC(5)=4, MAXEXC(7)=4, MAXEXC(8)=3, MAXEXC(10)=3,
```

```
      MSOL1(1,5)=1, MSOL1(2,5)=1, MSOL1(3,5)=1, MSOL1(4,5)=1,
      MSOL1(1,7)=1, MSOL1(2,7)=1, MSOL1(3,7)=1, MSOL1(4,7)=1,
      MSOL1(1,8)=1, MSOL1(2,8)=1, MSOL1(3,8)=1, MSOL1(4,8)=1,
      MSOL1(1,10)=1, MSOL1(2,10)=1, MSOL1(3,10)=1, MSOL1(4,10)=1,
      MSOL2(1,5)=1, MSOL2(2,5)=1, MSOL2(3,5)=1, MSOL2(4,5)=1,
      MSOL2(1,7)=1, MSOL2(2,7)=1, MSOL2(3,7)=1, MSOL2(4,7)=1,
      MSOL2(1,8)=1, MSOL2(2,8)=1, MSOL2(3,8)=1, MSOL2(4,8)=1,
      MSOL2(1,10)=1, MSOL2(2,10)=1, MSOL2(3,10)=1, MSOL2(4,10)=1,
      NUNIT=10000, NUNIT2=10000,
  /
```

INPUT(I), OUTPUT(0), WORK(W) file information

ifscmo(I), ifscer(I), ifscfi(I), ifsol1(I),
ifcom(O), ifscsy(O), iflabr(O), iflbra(O), iflabb(O), iflaba(O)
iflbt3(W)

##

#EGOP#

* Step EGOP, exponential(E) generation(G) of operators (OP) *

This step generates higher-order excitation operators up to sextuples for SAC-CI general-*R* and high-spin, by exponential generation scheme combined with perturbation selection.

Namelist Group -- &EGOP --

THRMA1,THRMA2
Thresholds for A(1) and A(2) operators, respectively, for exponential generation of higher-order terms by R=A*B
(Default: THRMA1=0.04, THRMA2=0.04)

Note
Only those A operators whose coefficients in the reference-CI are larger than THRMA1(2) are used for generating the higher-order linked operators R=A*B.

THMMA1,THMMA2
Thresholds for A(1) and A(2) operators, respectively, for exponential generation of higher-order terms by R=A*A*B
(Default: THMMA1=0.1, THMMA2=0.1)

THRMB1(KSTATE),THRMB2(KSTATE)
Thresholds for B(1) and B(2) operators, respectively, for

exponential generation of higher-order terms by R=A*B
(Default: THRMB1(KSTATE)=0.04, THRMB2(KSTATE)=0.04)

THMMB1(KSTATE),THMMB2(KSTATE)
Thresholds for B(1) and B(2) operators, respectively, for
exponential generation of higher-order terms by R=A*A*B
(Default: THMMB1(KSTATE)=0.1, THMMB2(KSTATE)=0.1)

ISELEG
Perturbation selection is done for higher-order linked terms.
=0 : without perturbation selection
=1 : with perturbation selection
(Default: 1)

ESELEG(KSTATE)
Energy threshold (in au) for perturbation selection
for the higher-order operators of KSTATE
(Default: 1.d-5)

** Note **
The reference functions for perturbation selection and
the type of selection is determined with CMAIN(KSTATE) and
ISEL(KSTATE), respectively. (See namelist &PRES)
ISEL(KSTATE) should be 1.

THRUI3(KSTATE),THRUI4(KSTATE),THRUI5(KSTATE),THRUI6(KSTATE) :
Threshold of generating unlinked integrals for the
unlinked operators R(3)=A(1)*B(2), A(2)*B(1), R(4)=A(2)*B(2),
R(5)=A(2)*A(2)*B(1), A(1)*A(2)*B(2), R(6)=A(2)*A(2)*B(2)
(Default: THRUI3(KSTATE)=0.1, THRUI4(KSTATE)=0.1,
THRUI5(KSTATE)=0.1, THRUI6(KSTATE)=0.1)

** Note **
For example, the R(5)=A(2)*A(2)*B(1) operator whose
products of reference CI coefficients a(2)*a(2)*b(1) are
larger than THRUI5(KSTATE) is used to generate the unlinked
terms R(5)*S(2).

MXRED
Unit of working space for storing selected operators
(Default: Automatically determined.)

** Note **
MXRED should be increased when the number of high-order
excitation operators exceed this limit.

MXRED2
Unit of working space for storing excitation operators
before perturbation selection

(Default: Automatically determined.)

TREMA1,TREMA2
Thresholds for A(1) and A(2) operators, respectively, for exponential generation of higher-order terms by R=A*B of reference-EGCI.
(Default: TREMA1=0.1, TREMA2=0.1)

TREMB1(KSTATE),TREMB2(KSTATE)
Thresholds for B(1) and B(2) operators, respectively, for exponential generation of higher-order terms by R=A*B of reference-EGCI.
(Default: TREMB1(KSTATE)=0.1, TREMB2(KSTATE)=0.1)

IPRINT: Level of printing, see &PRES for details.
(Default: IPRINT=0)

Sample input

```
&EGOP
   ESELEG(1)=5.d-6, ESELEG(2)=5.d-6, ESELEG(3)=5.d-6,
   THRMA1=0.04, THRMA2=0.04, THMMA1=0.1, THMMA2=0.1,
   THRMB1(1)=0.04, THRMB1(2)=0.04, THRMB1(3)=0.04,
   THRMB2(1)=0.04, THRMB2(2)=0.04, THRMB2(3)=0.04,
   THMMB1(1)=0.1, THMMB1(2)=0.1, THMMB1(3)=0.1,
   THMMB2(1)=0.1, THMMB2(2)=0.1, THMMB2(3)=0.1,
   THRUI3(1)=0.1, THRUI4(1)=0.1, THRUI5(1)=0.1, THRUI6(1)=0.1,
   ISELEG=1, MXRED=10000, MXRED2=5000, IPRINT=0
/
```

INPUT(I), OUTPUT(0), WORK(W) file information

```
ifcom(I),    ifscmo(I), ifscer(I), ifscsy(I),
iflabr(I), iflbra(I), iflabb(I), iflaba(I), ifsol1(I), ifsol2(I),
iflabe(O),
iflbt1(W), iflbt2(W), iflbt3(W)
```

##

---

* Step MEGI * #MEGI#

Hamiltonian matrix, overlap matrix, and unlinked integrals for SAC-CI general-*R* and high-spin calculations.

Input

Namelist Group -- &MEGI --

** Note **
(1) Thresholds of unlinked integrals are the same as in ULINT.
(CMAX, CMAXES, and CMAXED)

(2) For generating the unlinked terms R(x)*S(2) for higher-order linked excitation operators R(x) (x=3,...,6), such R(x) were already selected in #EGOP# using THRUI3(KSTATE) - THRUI6(KSTATE).

THRINT : Threshold of integrals stored
(Default : thrint=1.d-8)

IPRINT: Level of printing, see &PRES for details.
(Default: IPRINT=0)

Notes:
(a) "ISTEP": shows the function of the step #MEGI# and is controlled by the step #SUPER97#.

istep = 1 : integrals for reference-CI
= 2 : integrals for single and double CI
= 5 : linked integrals for SAC-CI (general-*R*) or EGCI
= 6 : unlinked integrals for SAC-CI (general-*R*), and SAC-CI (high-spin)

(b) Selection of the excitation operator for unlinked term also depends on input data "CSPIN" defined in namelist &PRES. Namely, when cspin=1, the spin function of the excitation operator R(x) for unlinked term spans complete spin space.

(c) Unlinked terms which are redundant with linked terms can be neglected, so that the overlap matrix between linked and unlinked term is absent.

(d) Integral evaluations of some linked terms, H11, H21, and H22 and unlinked terms, H13, H23, and H24, are performed by using the same subroutines as in the SD-*R* part for kstate=1 to 4.

(f) When NTGENH=1 is selected in &GHPRES, CMAXEH is active.

CMAXEH : Threshold for selection of R(3) operators in SAC-CI.
If a R(3) coefficient is larger than CMAXEH,
it is included in the R(3)*S(I) terms.
The R(3) coefficients for selection are obtained

from small CI result file.
(Default: CMAXEH=0.1)

Sample input

&MEGI
CMAX=0.001, CMAXES=0.05, CMAXED=0.05, THRINT=1.d-8, IPRINT=0, /

INPUT(I), OUTPUT(0), WORK(W) file information

ifcom(I), ifscmo(I), ifscer(I), ifscsy(I),

istep	Excitation operators	Hamiltonian matrix	overlap matrix	unlinked integrals	solutions
1	iflabr(I)	ifhmx1(O)	ifsmx1(O)	- - -	- - -
2	iflabb(I)	ifhmx2(O)	ifsmx2(O)	- - -	- - -
4	iflbra(I)	ifhmre(O)	ifsmre(O)	- - -	- - -
5	iflabe(I)	ifhmx3(O)	ifsmx3(O)	- - -	- - -
6	iflabe(I) iflabs(I)	- - -	- - -	ifumx3(I)	ifsol1(I) ifsol2(I) ifsols(I)

##

* step GHDENS * #GHDENS#

This step calculates density matrix, natural orbitals,
transition density matrix, and spin density matrix for SAC-CI
(general-*R*) and SAC-CI (high-spin) states.

Literature :
H. Nakatsuji and K. Hirao, Int. J. Quantum Chem. 20, 1301 (1981)

Namelist Group -- &GHDENS --

CMAX, CR1MAX, ISSCIG, KSTATT, ISYMTT, ISOLTT, ILEFT, THRECCC, IPRINT
Same as in Namelist &DENS

Sample input

&GHDENS CMAX=1.d-3, CR1MAX=0.1, IPRINT=0, /

INPUT(I), OUTPUT(0), WORK(W) file information

ifcom(I), ifsol3(I: SAC-CI-V), ifsl3n(I: SAC-CI-NV),
ifsols(I), iflabe(I), iflabs(I),
ifdens(O), iftden(O)

II-D. SAC/SAC-CI Analytical Energy Gradient Part

Availability and Restriction

See I-D-5.

Structure

See I-D.

Notice

Some non-standard options of the related steps shown below do not work in the gradient step.

```
OPTIONS NOT YET IMPLEMENTED IN GRADIENT PART
============================================
TERM1,TERM2,TERM3 in &ULINT
IN2ND in &SCIV, ISCRPT in &SCINV
SCRPTS in &DAS, &DNAS
all options in &FOCK and NONHF in &CNTL
============================================
```

##

* Step CPSAC Z-vector Iterative * #ZVECIT#

Link 923

In this step, CPSAC Z-Vector equations are solved iteratively.

For Keyword, see USERS' REFERENCE.
For geometry optimization, use Keyword Opt.
For analytical energy gradients at single point, use Keyword Force.

Namelist input is not available.

##

In this step, 1-particle and 2-particle effective density matrices (EDMs) of SAC/SAC-CI singlet, triplet, ionized, electron attached, quartet, quintet, sextet and septet state are constructed.

For IOp, see PROGRAMMER'S REFERENCE.

There is no Keyword to control this step.
Namelist input is not available.

Input example 1

SAC-CI-NV for 1st triplet excited state of symmetry 2 without perturbation selection.

```
#P SACCI(FullAC,Singlets(0,1,0,0,0,0,0,0),NoSelection,
    TargetState=Triplet,TargetSymmetry=1,TargetRoot=1)
    /3-21G Opt
```

(molecular specification)

Input example 2

SAC-CI-V for 1st (lowest) singlet excited state with perturbation selection in Pipek and Mezey's LMO basis.

```
#P SACCI(FullAC,Variational,Singlets(1),LMO(PM),
    TargetState=Singlet,TargetSymmetry=1,TargetRoot=1)
    /3-21G Opt NoSymmetry
```

(molecular specification)
Input example 3

SAC-CI-V general-*R* for 2nd iondoublet state of symmetry 3

```
#P SACCI(FullAC,Variational,GeneralR,Iondoublets=(1),
    TargetState=Iondoublet,TargetSymmetry=3,TargetRoot=2)
    /3-21G Opt
```

See also instructions for GSUM method in Part II.

Part III. Controlling Files in SAC-CI SD-*R*, SAC-CI General-*R*, High-Spin, and SAC/SAC-CI Energy Gradient Calculations

(See Tables 1-3 of Part I-D-1,3)

File numbers, contents and their usages are described in detail.

III-A. File numbers of SAC/SAC-CI SD-*R* calculation

List of file numbers and contents of files generated in SAC/SAC-CI SD-*R* calculations. Subroutine FileIO is used for I/O of these files. Indices 'i' and 'j' refer to kstate and ksym, respectively, in the File name' and 'File numbers' of the following table.

These file numbers are defined in Subroutine Scarrd and are referred through the common block ifscfn etc.

```
common /ifscfn/ ifsccm,ifscmo,ifscer,ifscfi,ifscsi,ifscsy,ifsciw,
.     ifsh24,       ifsh02,      ifscka(4),   ifscgk(4),
.     ifschh(9,4),  ifscss(9,4), ifscit(9,4),  ifscrc(9,4), ifscun(9,4),
.     ifsckx(9,4),  ifscsv(9,4),ifscsn(9,4),ifscno(9,4),          ifsctd(9,4),
.     ifscul,ifscgr(9,4)
common /ifscf2/ ifsck1(4),ifsch1(9,4),ifscs1(9,4)
common /ifscf3/ ifflag
common /ifscf5/ ifsccg
common /ifscf7/ ifscc1
common /ifififf/ ififcm
```

The files containing information of the state for which the gradients are calculated are gathered into "permanent" region of RWF, to avoid that they are cleared-up at the end of execution of each Overlay or Link. EGSym and EGState denotes ISYM and KSTATE for the target state of gradient calculation, respectively.

Access to each file is shown as <O:output/I:input/W:working unit>

File name	File numbers	Contents and structure (C2v case)
### read-write file ###		
ifscer	3503	E : Orbital energies R : MO electron repulsion integrals (MOERI) Llim : Lower limit of active MOs Iulim: Upper limit of active MOs Symmetrically non-zero MOERI's are

stored.
(E(i),i=1,Nbf)
Nmo,Nbasis,Llim,Iulim, (itype)
(R(i),i=1,N)
<O:BPRES/I:PRES,CIMX,ULINT,ZVECIT>

ifscsy 3506 Information for symmetric reduction of molecular integrals
<O:BPRES/I:PRES,CIMX,ULINT,ZVECIT,EDM>

ifsh24 301 Hamiltonian matrix element
<S(I)|H|S(I)*S(I)>
and overlap matrix element
<S(2)|S(1)*S(1)>
for SAC wave function
<O:ULINT/I:SAC,DSAC,ZVECIT>

ifsh02 3509 Hamiltonian matrix element
<0|H|S(1)*S(1)>
for SAC wave function
<O:ULINT/I:SAC,DSAC>

ifschh(j,i) (i+6)*500+ 20+j Hamiltonian matrix elements between linked terms
i=1,j=1 G,E ...HII...;...H01,H02...;
...I,J...;...HIJ...;...
else E ...HII...;...I,J...;
...HIJ...;...
<O:CIMX/I:SCIV,SCINV,DAS,DNAS,ZVECIT,EDM>

ifscun(j,i) (i+6)*500+ 60+j Unlinked terms containing
<R(I)|H|R(I)*S(I)> for SAC-CI-V and NV
E ...I,J...;...UIJ...;...
<O:ULINT/I:SCIV,SCINV,DAS,DNAS>

```
#########################
###     check point file     ###
#########################
```

ifscc1 340 NAT34 information

ifsccg 341 General computational information in Gsum step
File structure is identical to ifsccm.
<O:GSUM/I:ALL STEPS>

ifscgk(i) 342+i Excitation operators in Gsum step
File structure is identical to ifscka(i)
<O:GSUM/I:ALL STEP>

ifscgr(j,i) 340+i*10+j Flags for R1- and R2- operators for
calculating unlinked integrals in Gsum

<O:GSUM/I:ALL STEP>

ifscul 342 Flags for S2- operators for calculating unlinked terms

<O:GSUM/I:ULINT,ZVECIT,EDM>

ifflag 3500 Job status of SAC/SAC-CI calculation

<O/I:SUPER>

ifsccm 3501 General computational information

<O:PRES/I:ALL STEPS>

ifscmo 3502

```
C     : Molecular orbitals
E     : Orbital energies
Fmx   : Fock matrix
Nbf   : Number of active space
Ncore : Number of core MOs
Mosym : Symmetry of MOs
Nbasis: Number of AOs in SCF
Nmo   : Number of MOs in SCF
    ((C(i,j),i=1,Nbasis),j=1,Nmo)
    (E(i),i=1,Nmo)
    (Fmx(i),i=1,Nbf*(Nbf+1)/2)
    Nbf,Ncore,(Mosym(i),i=1,Nbf)
```

<O:BPRES/I:PRES,CIMX,ULINT,DENS,EDM>

ifscfi 3504 Information of MOERI file
nferi,nblk,kount,nunit

<O:BPRES/I:PRES,CIMX,ULINT,ZVECIT,EDM>

ifscsi 3505 Parameters for array sizes used in dynamical allocation of memory
The contents of parameters are shown in #SUPER97#.
(nsp(i),i=1,18)

<O:BPRES/I:ALL STEPS>

ifscka(i) (i+6)*500+ 10 Excitation operators after configuration selection:
G(ground), E(excited), KABL1(singles),KABL2(doubles)

```
i=1     A1 G     ...KABL1...;...KABL2...;
           E     ...KABL1...;...KABL2...;
        A2    E        ...KABL1...;...KABL2...;
        B1    E        ...KABL1...;...KABL2...;
        B2    E        ...KABL1...;...KABL2...
else     A1   E        ...KABL1...;...KABL2...;
        A2    E        ...KABL1...;...KABL2...;
        B1    E        ...KABL1...;...KABL2...;
        B2    E        ...KABL1...;...KABL2...
```

<O:PRES/I:ALL STEPS>

```
ifscss(j,i)     (i+6)*500+ 30+j          Overlap matrix elements between linked
                                                 G,E      ...SII...;..I,J...;...SIJ...
<O:CIMX/I:SCIV,SCINV,DAS,DNAS,ZVECIT,EDM>

ifscit(j,i)     (i+6)*500+ 40+j          Initial vectors (usually SECI vectors)
                                         and HII (for normalized |I>)
                                                       G        ...HII...;...VECG...
                                                       E        ...HII...;...VECE1..;
                                                       ...VECE2...;...
<O:PRES/I:PRES,CIMX,CID,ULINT,SAC,DSAC,SCIV,SCINV,DENS,ZVECIT,EDM>

ifscrc(j,i)     (i+6)*500+ 50+j          CISD energy and coefficient as
                                          Isol,Icond,Lamb,(W(i),i=1,Ndt):...
                                             Isol     : Solution number.
                                             Icond    : Condition code
                                               1 ... Converged with density and
                                                       energy criterion.
                                               2 ... Converged with energy
                                                       criterion.
                                               3 ... Not converged.
                                             Lamb     : CISD energy.
                                             W        : CISD coefficient.
<O:CID/I:ULINT,SAC,DSAC,ZVECIT,EDM>

ifsckx(j,i)     (i+6)*500+120+j          Flags for R1- and R2- operators for calculating unlinked
                                         integrals
<O:ULINT/I:DENS,ZVECIT,EDM>

ifscsv(j,i)     (i+6)*500+ 70+j          i=1,j=1 : SAC-NV energy and solution
                                           Temet, (Cm(i),i=1,Ndt)
                                             Temet  : SAC-NV correlation energy
                                             Cm     : SAC-NV coefficients

                                         else : SAC-CI-V energies and
                                                coefficients
                                           Isol,Icond,Lamb,(W(i),i=1,Ndt);...
                                             Isol,Icond       : same as ifscrc
                                             Lamb     : SAC-CI-V energy.
                                             W        : SAC-CI-V coefficient.
<O:SCIV,DAS/I:DENS,ZVECIT,EDM>

ifscsn(j,i)     (i+6)*500+ 80+j          i=1,j=1 : same as ifscsv(1,1)

                                         else : SAC-CI-NV energies and
                                                coefficients
                                           Isol,Icond,Lamb,(W(i),i=1,Ndt);...
                                             Isol,Icond       : same as ifscrc
                                             Lamb     : SAC-CI-V energy.
                                             W        : Right SAC-CI-NV coefficient.
```

```
<O:SCINV,DNAS/I:DENS,ZVECIT,EDM>

ifscno(j,i)    (i+6)*500+100+j          Occupation numbers and natural orbitals
                                          Kstate,Isym,Ist,(Aocc(i),i=1,Nmo)
                                         ((W(i,j),i=1,Nbf),j=1,Nmo):...
                                         Ist      : Number of state
                                         Aocc     : Occupation numbers
                                         W        : Natural orbitals
<O:DENS/I:PROP>

ifsctd(j,i)    (i+6)*500+110+j          Transition densities or Spin densities
                                         (i) Transition density
                                                  Kstate,Isym,Ist,Iden,
                                                  ((W(ii,jj),ii=1,Nbf),jj=1,Nmo):...
                                         (ii) Spin density
                                                  ((W(ii,jj),ii=1,Nbf),jj=1,Nmo):...
<O:DENS/I:PROP>

###########################
###   scratch file (xxx.scr)   ###
###########################

ifsciw         3507                     Work unit
<W:PRES,SCIV,SCINV>

ifsck1(i)      (i+6)*500+ 10            Work unit for saving excitation operators
                                        File structure is identical to ifscka(i)
<W:PRES/I:CIMX>

ifsch1(j,i)    (i+6)*500+ 20+j          Work unit for saving diagonal elements
                                        of Hamiltonian matrix
<O:PRES/I:CIMX>

ifscs1(j,i)    (i+6)*500+ 30+j          Work unit for saving diagonal elements
                                        of Overlap matrix
<O:PRES/I:CIMX>
```

III-B. File numbers of SAC/SAC-CI general-*R* and high-spin calculation

List of file numbers and contents of files generated in SAC/SAC-CI general-*R* and high-spin calculations. Subroutine FileIO is used for I/O of these files. Indices 'i' and 'j' refer to kstate and ksym, respectively, in the 'File name' and 'File numbers' of the following table.

These file numbers are defined in Subroutine Arrghp and are referred through the common block Ghfile etc.

```
common /ghfile/ ifcom,ifmo,iferi,iflabb(8),iflaba(8),iflabs,
.     iflabr(8),iflabe(8),iflbre(8),iflbt1(8),iflbt2(8),iflbt3(8),
.     ifhmx1(8),ifhmx2(8),ifhmx3(8),ifhmre(8),ifsmx1(8),ifsmx2(8),
```

. ifsmx3(8),ifsmra(8),ifsmxa(8),ifsmre(8),ifumx3(8),ifusx3(8),
. ifsol1(8),ifsl1a(8),ifsol2(8),ifsl2a(8),
. ifsol3(8),ifsl3n(8),ifslre(8),ifdens(8),iftden(8),ifsols

Access to each file is shown as <O:Output/I:Input/W:Working unit>

```
---------------   -------------------------   ------------------------------------------------------------------------------
File name         File numbers                  Contents and structure (C2v case)
---------------   -------------------------   ------------------------------------------------------------------------------
#########################
###     read-write file       ###
#########################

  iferi           3503                        MOERI file (same as ifscer of SD-R)
  (IOERI)                                     Used in ZVecIt

  ifscsy         3506                         Same as SD-R
  (IOSCSY)                                    Used in ZVecIt
    <I:MEGI,ZVECIT>

  ifhmx1(j)    (i+6)*500+360+j                Hamiltonian matrix elements of reference-CI
                                                ..HII..;..I,J..;..HIJ..;..I,J..;
                                                ..HIJ..;...
    <O:MEGI/I:DAS>

  ifhmre(j)     (i+6)*500+470+j               Hamiltonian matrix elements of reference-EGCI
                                                ..HII..;..I,J..;..HIJ..;..I,J..;
                                                ..HIJ..;...
    <O:MEGI/I:DAS>

  ifhmx2(j)     (i+6)*500+400+j               Hamiltonian matrix elements of singles and doubles
                                                ..HII..;..I,J..;..HIJ..;..I,J..;
                                                ..HIJ..;...
  (IOHMX2)  ifhmx2(EGKSym)                    Used in ZVecIt and Ov.11
    <O:MEGI/I:SCIV,SCINV,DAS,DNAS,ZVECIT,EDM>

  ifhmx3(j)     (i+6)*500+ 20+j               Hamiltonian matrix elements of triples and higher
                                                ..HII..;..I,J..;..HIJ..;..I,J..;
                                                ..HIJ..;...
  (IOHMX3) ifhmx3(EGKSym)                     Used in ZVecIt and Ov.11
    <O:MEGI/I:SCIV,SCINV,DAS,DNAS,ZVECIT,EDM>

  ifumx3(j)     (i+6)*500+ 60+j               Hamiltonian matrix elements between linked and unlinked
                                              terms of SAC-CI high-spin and general-R
                                                ..I,J..;..UIJ..;..I,J..;..UIJ..;...
    <O:MEGI/I:SCIV,SCINV,DAS,DNAS>

  ifusx3(j)     (i+6)*500+340+j               Overlap matrix elements between linked and unlinked
```

```
                                        terms of SAC-CI general-R
                                          ..I,J..;..UIJ..;..I,J..;..UIJ..;...
    <O:MEGI/I:SCIV,SCINV,DAS,DNAS>

#########################
###     check point file     ###
#########################

   ifcom        3507                    General computational information of
                                        SAC-CI high-spin and general-R
   (IOFCOM)                             Used during geometry optimization
    <O:GHPRES/I:ALL STEPS>

   ifmo         3502                    MO file (same as ifscmo in SD-R)
   (IOMO)                               Used in ZVecIt
    <I:MEGI,GHDENS,ZVECIT>

   ifscfi       3504                    Same as SD-R
   (IOSCFI)                             Used in ZVecIt
    <I:MEGI,GHDENS,ZVECIT>

   iflabb(j)    (i+6)*500+390+j         Single and double excitation operators (A- and B-operators)
                                            ..Singles..;..Doubles..
   (iflaba(j)                           for singlet-type operators)
   (IOSCKB(j))                          Used during geometry optimization
    <O:GHPRES/I:EGOP,MEGI,SCIV,SCINV,DAS,DNAS,ZVECIT>

   iflabr(j)    (i+6)*500+350+j         Single and double excitation operators of reference-CI
                                            ..Singles..;..Doubles..
   (iflbra(j)                           for singlet-type operators)
   (IOSCKR(j))                          Used during geometry optimization
    <O:GHPRES/I:EGOP,MEGI,DAS,ZVECIT>

   iflabe(j)     (i+6)*500+ 10+j        Excitation operators of SAC-CI high-spin and general-R
                                            ..Singles..;..Doubles..;..Triples..;
                                            ...;...;...
   (IOSCKA(j)) ifscka(j)                Used during geometry optimization
   (IOLABE)  iflabe(EGKSym)             Used in ZVecIt and Ov.11
    <O:EGOP/I:MEGI,SCIV,SCINV,DAS,DNAS,ZVECIT,EDM>

   iflbre(j)    (i+6)*500+460+j         Excitation operators of reference-EGCI (small active space)
                                            ..Singles..;..Doubles..;..Triples..;
                                            ..Quadruples..
    <O:EGOP/I:EGOP,MEGI>

   ifsmx1(j)    (i+6)*500+370+j         Overlap matrix elements of reference-CI
                                            ..SII..;..I,J..;..SIJ..
   (ifsmra(j)                           for singlet-type operators)
    <O:MEGI/I:GHPRES,EGOP,DAS>
```

```
ifsmre(j)     (i+6)*500+480+j          Overlap matrix elements of reference-EGCI
                                           ..SII..;..I,J..;..SIJ..;..I,J..;
                                           ..SIJ..
  <O:MEGI/I:EGOP,DAS>

ifsmx2(j)     (i+6)*500+410+j          Overlap matrix elements of singles and doubles
                                           ..SII..;..I,J..;..SIJ..
(ifsmxa(j)                             for singlet-type operators)
  <O:MEGI/I:EGOP,SCIV,SCINV,DAS,DNAS>

ifsmx3(j)     (i+6)*500+ 30+j          Overlap matrix elements of triples and highers
                                           ..SII..;..I,J..;..SIJ..;..I,J..;
                                           ..SIJ..
  <O:MEGI/I:SCIV,SCINV,DAS,DNAS>

ifsol1(j)     (i+6)*500+380+j          Eigenvalues and eigenvectors of reference-CI
                                           ..E(i)..;..VEC1..;..VEC2..;...
(ifsl1a(j)                             for singlet states)
  <O:DAS/I:GHPRES,EGOP,SCIV>

ifslre(j)     (i+6)*500+470+j          Eigenvalues and eigenvectors of reference-EGCI
                                           ..E(i)..;..VEC1..;..VEC2..;...
  <O:DAS/I:EGOP>

ifsol2(j)     (i+6)*500+420+j          Eigenvalues and eigenvectors of SD-CI
                                           ..E(i)..;..VEC1..;..VEC2..;...
(ifsl2a(j)                             for singlet states)
  <O:SCIV,DAS/I:EGOP,MEGI,SCIV>

ifsol3(j)     (i+6)*500+ 70+j          Eigenvalues and eigenvectors of
                                       SAC-CI-V high-spin and general-R
                                           ..E(i)..;..VEC1..;..VEC2..;...
(IOSOL3)      ifsol3(EGKSym)           Used in ZVecIt and Ov.11
  <O:SCIV,DAS/I:GHDENS,ZVECIT,EDM>

ifsl3n(j)     (i+6)*500+ 80+j          Eigenvalues and eigenvectors of
                                       SAC-CI-NV high-spin and general-R
                                           ..E(i)..;..VEC1..;..VEC2..;...
(IOSL3N)      ifsl3n(EGKSym)           Used in ZVecIt and Ov.11
  <O:SCINV,DNAS/I:GHDENS,ZVECIT>

ifdens(j)     (i+6)*500+100+j          Occupation numbers and natural orbitals
                                           same as ifscno
  <O:GHDENS>

iftden(j)     (i+6)*500+110+j          Density matrix and transition density matrix
                                           same as ifsctd
  <O:GHDENS>
```

ifini3(j)	(i+6)*500+490+j	Initial vectors for iterative diagonalization
<O:SCIV/I:SCIV>		
iflabs	3497	Excitation operators of SAC ground state (transferred from SAC-CI SD-*R*)
(IOLABS)	ifscgk(1)	Used in ZVecIt and Ov.11
<I:MEGI,SATEI,ZVECIT,EDM>		
ifsols	3498	SAC-NV solution (transferred from SAC-CI SD-*R*)
(IOSOLS)		Used in ZVecIt and Ov.11
<I:MEGI,SATEI,ZVECIT>		
ifsss	3499	Overlap matrix of SAC (transferred from SAC-CI SD-*R*)
(IOSMXS)		Used in ZVecIt and Ov.11
<I:MEGI,SATEI,ZVECIT>		

```
###########################
###   scratch file (xxx.scr)   ###
###########################
```

ifscwk(4)	3521-3524	Work unit
<I:EGOP,SCIV,SCINV>		
ifscwi(8)	3511-3518	Work unit
<I:EGOP,SCIV,SCINV>		
iflbt1(j)	(i+6)*500+430+j	Work unit for saving A-operators and maximum absolute values of SD-CI coefficients ..Singles..;..Doubles..; ..Max(Abs(Vec))..
<W:EGOP>		
iflbt2(j)	(i+6)*500+440+j	Work unit for saving B-operators and maximum absolute values of SD-CI coefficients ..Singles..;..Doubles..; ..Max(Abs(Vec))..
<W:EGOP>		
iflbt3(j)	(i+6)*500+450+j	Work unit for saving reference excitation operators for perturbation selection ..Singles..;..Doubles..
<W:GHPRES,EGOP>		

III-C. File numbers of SAC/SAC-CI SD-*R* energy gradient calculation

In Link 923, many files (controlled mainly by /ifscfn/) are generated as 'volatile' files. They are deleted automatically at the end of the Link. Because effective density matrices (EDMs) are constructed by different program (Link), it is necessary to save selected information of SAC and SAC-CI wavefunctions, e.g. excitation labels, eigenvectors, and indices of non-zero elements of H matrices considered in the calculation. This is done through 'permanent' rwf's listed in Link 1, and copying files to the permanent rwf's is done at the end of execution of Link 923, by subroutine SGrPak. In EDM calculations, files packed into the permanent rwf's are treated as logical subfiles available by FileIO. Some types of data, mainly excitation labels, are returned to Link 923 at the beginning of the execution to keep geometry independent information during optimization.

III-D. File numbers of SAC-CI general-*R* and high-spin energy gradient calculation

List of file numbers and contents of files generated in SAC/SAC-CI general-*R* and high-spin gradient calculations. Subroutine FileIO is used for I/O of these files. Index 'j' refer to ksym (j=1,8), in the 'File name' and 'File numbers' of the following table. EGSym refer to target symmetry in the gradient calculation.

File numbers are defined in Subroutine sdtgh1(GHPRES) and ZGHfio (ZVECIT) and are mainly referred through two common blocks /ghfil0/ and /GGHFIL/.

Access to each file is shown as <O:output/I:input/W:working unit>

File name	Contents and structure

Common block /ghfil0/

File Numbers transferred from SAC-CI SD-*R*

IOSH24	ifsh24
<O:ULINT/I:SAC,DSAC,ZVECIT>	
IOSCUL	ifscul
<O:GSUM,GHPRES/I:ULINT,ZVECIT,EDM>	
IOLABS	ifscgk(1)
IOHMXS	ifschh(1,1)
<O:CIMX,GHPRES/I:ZVECIT,EDM>	

File Numbers defined/transfered in GHPRES or MEGI

IOSCGR(j)	Flags for R- operators for calculating unlinked integrals
IORdR3(j)	Flags for redundant terms between linked and unlinked terms for R(3)
IORdR4(j)	Flags for redundant terms between linked and unlinked terms for R(4)
IORdRH(j)	Flags for redundant terms between linked and unlinked terms for

more higher-order operators.

<O:MEGI/I:MEGI,ZVECIT>

IOSCKR(j)	iflabr(KSym)
IOSCKB(j)	iflabb(KSym)
IOSCKA(j)	iflabe(KSym)

<O:ZVECIT/I:GHPRES,SCIV,DAS,DNAS,MEGI,ZVECIT>

IOFCOM	ifcom

<O:GHPRES/I:GHPRES>

Common block /GGHFIL/

File Numbers defined/transfered in ZVecIt (Subroutine ZGHfio)

IOMO	ifmo
IOERI	iferi
IOSCSY	ifscsy
IOSCFI	ifscfi

<O:/I:ZVECIT>

IOSH24	JOSH24
IOSCUL	JOSCUL
IOLABS	JOLABS
IOHMXS	JOHMXS
IOHMX2	ifhmx2(EGKSym)
IOHMX3	ifhmx3(EGKSym)
IOMO	ifmo
IOSOLS	ifsols
IOSMXS	ifsss
IOSOL3	ifsol3(EGKSym)
IOSL3N	ifsl3n(EGKSym)
IOLABE	JOSCKA(EGKSym)
IOSCKX	JOSCGR(EGKSym)
IORdR3	JORdR3(EGSym)
IORdR4	JORdR4(EGSym)
IORdRH	JORdRH(EGSym)
IBucZv	CPSAC Z-vectors

<O:/I:ZVECIT,EDM>

IOSCSR	Information of Common blocks

<O:ZVECIT/I:EDM>

Part IV Control of SAC-CI Keyword Options in L1 of Gaussian

IV-A. Input Style of Keyword Option

The options in the SAC-CI keywords are given on a route card as

SAC-CI=(keyword1, keyword2, keyword3,,,,).

There are two kinds of keywords in the SAC-CI method. One is global keyword, which affects all spin-multiplicities, and the other is state-specific keyword, which is given for a specified state and affects only that state. The global and state-specific keywords are given as

```
SAC-CI=(keyword1, keyword2,,, Singlet=(keyword3, keyword4,,,)
                              Triplet=(keyword5, keyword6,,,)
                                   ,,,,
                              Sextet=(keyword7, keyword8,,,,)
                              Septet=(keyword9,  keyword10,,,,)    ).
```

IV-B. Storage and Flow of Keyword Options

These keyword options are parsed in #ParSAC# of L1.F, and are translated into integers or floating-point numbers. They are saved in an array of L1.F. At the end of L1.F (#SavSCI#), this array is saved onto RW-File (permanent address #734). This array is read and used in #SACTrIOp# of 000sacci1.f (Link923) to make MyIOp, which is actually utilized for controlling a job of SAC-CI. The flow of the keyword options is summarized as below.

```
SAC-CI options    ----->    Array in core    ------->    Array in RWF    --------->    MyIOp
                     #PrcSAC#                  #SavSCI#                      #SACTrIOp#
|--------------------------- L1 ----------------------------|    |-----------------Link923-----------------|
```

For details, see #PrcSAC#, #SavSCI#, #PrcSC1#, #PrcSC2# in L1.F, and #SACTrIOp# in 000sacci1.f (L923.F).

IV-C. Array for Keyword Options

Table Array containing information parsed from SAC-CI keyword options

Array Element and size	SAC-CI Keywords and sub-keywords	Comment Translation (--->)
Dimension ISACCI(10,8)		
	==== Singlet State ====	
ISACCI(1,1)	Singlet=Nstate=N	Number of Solutions for singlet states
ISACCI(2,1)	Singlet=Nstate=(N-------)	
ISACCI(3,1)	Singlet=Nstate=(-N------)	
ISACCI(4,1)	Singlet=Nstate=(--N-----)	

```
ISACCI(5,1)        Singlet=Nstate=(---N----)
ISACCI(6,1)        Singlet=Nstate=(----N---)
ISACCI(7,1)        Singlet=Nstate=(-----N--)
ISACCI(8,1)        Singlet=Nstate=(------N-)
ISACCI(9,1)        Singlet=Nstate=(-------N)
             ==== Triplet State ====
ISACCI(1,1)        Triplet=Nstate=N                    Number of Solutions for triplet states
ISACCI(2,2)        Triplet=Nstate=(N-------)
ISACCI(3,2)        Triplet=Nstate=(-N------)
ISACCI(4,2)        Triplet=Nstate=(--N-----)
ISACCI(5,2)        Triplet=Nstate=(---N----)
ISACCI(6,2)        Triplet=Nstate=(----N---)
ISACCI(7,2)        Triplet=Nstate=(-----N--)
ISACCI(8,2)        Triplet=Nstate=(------N-)
ISACCI(9,2)        Triplet=Nstate=(-------N)
             ==== CationDoublet ====             Number of Solutions for cation-doublet
ISACCI(1,3)        CationDoublet=Nstate=N
ISACCI(2,3)        CationDoublet=Nstate=(N-------)
ISACCI(3,3)        CationDoublet=Nstate=(-N------)
ISACCI(4,3)        CationDoublet=Nstate=(--N-----)
ISACCI(5,3)        CationDoublet=Nstate=(---N----)
ISACCI(6,3)        CationDoublet=Nstate=(----N---)
ISACCI(7,3)        CationDoublet=Nstate=(-----N--)
ISACCI(8,3)        CationDoublet=Nstate=(------N-)
ISACCI(9,3)        CationDoublet=Nstate=(-------N)
             ==== AnionDoublet ====
ISACCI(1,4)        AnionDoublet=Nstate=N               Number  of Solutions for anion-doublet
ISACCI(2,4)        AnionDoublet=Nstate=(N-------)
ISACCI(3,4)        AnionDoublet=Nstate=(-N------)
ISACCI(4,4)        AnionDoublet=Nstate=(--N-----)
ISACCI(5,4)        AnionDoublet=Nstate=(---N----)
ISACCI(6,4)        AnionDoublet=Nstate=(----N---)
ISACCI(7,4)        AnionDoublet=Nstate=(-----N--)
ISACCI(8,4)        AnionDoublet=Nstate=(------N-)
ISACCI(9,4)        AnionDoublet=Nstate=(-------N)
             ==== Quartet ====
ISACCI(1,5)        Quartet=Nstate=N                    Number of Solutions for quartet states
ISACCI(2,5)        Quartet=Nstate=(N-------)
ISACCI(3,5)        Quartet=Nstate=(-N------)
ISACCI(4,5)        Quartet=Nstate=(--N-----)
ISACCI(5,5)        Quartet=Nstate=(---N----)
ISACCI(6,5)        Quartet=Nstate=(----N---)
ISACCI(7,5)        Quartet=Nstate=(-----N--)
ISACCI(8,5)        Quartet=Nstate=(------N-)
ISACCI(9,5)        Quartet=Nstate=(-------N)
ISACCI(1,6)        Quintet=Nstate=N
             ==== Quintet ====
ISACCI(2,6)        Quintet=Nstate=(N-------)           Number of Solutions for quintet states
ISACCI(3,6)        Quintet=Nstate=(-N------)
```

```
ISACCI(4,6)        Quintet=Nstate=(--N-----)
ISACCI(5,6)        Quintet=Nstate=(---N----)
ISACCI(6,6)        Quintet=Nstate=(----N---)
ISACCI(7,6)        Quintet=Nstate=(-----N--)
ISACCI(8,6)        Quintet=Nstate=(------N-)
ISACCI(9,6)        Quintet=Nstate=(-------N)
              ==== Sextet ====
ISACCI(1,7)        Sextet=Nstate=N                        Number of Solutions for sextet states
ISACCI(2,7)        Sextet=Nstate=(N-------)
ISACCI(3,7)        Sextet=Nstate=(-N------)
ISACCI(4,7)        Sextet=Nstate=(--N-----)
ISACCI(5,7)        Sextet=Nstate=(---N----)
ISACCI(6,7)        Sextet=Nstate=(----N---)
ISACCI(7,7)        Sextet=Nstate=(-----N--)
ISACCI(8,7)        Sextet=Nstate=(------N-)
ISACCI(9,7)        Sextet=Nstate=(-------N)
              ==== Septet ====
ISACCI(1,8)        Septet=Nstate=N                        Number of Solutions for septet states
ISACCI(2,8)        Septet=Nstate=(N-------)
ISACCI(3,8)        Septet=Nstate=(-N------)
ISACCI(4,8)        Septet=Nstate=(--N-----)
ISACCI(5,8)        Septet=Nstate=(---N----)
ISACCI(6,8)        Septet=Nstate=(----N---)
ISACCI(7,8)        Septet=Nstate=(-----N--)
ISACCI(8,8)        Septet=Nstate=(------N-)
ISACCI(9,8)        Septet=Nstate=(-------N)

ISACCI(10,1)       TargetState=SpinState=
                       Singlet/Triplet/CationDoublet/AnionDoublet/
                       Quintet/Quartet/Sextet/Septet      --->   1/2/3/4/5/6/7/8
ISACCI(10,2)       TargetState=Symmetry=N
ISACCI(10,3)       TargetState=Root=N
ISACCI(10,4)       MaxItDiag=N
ISACCI(10,5)       WithHF/WithoutHF                       --->   1/2
ISACCI(10,6)       MaxR2Op=N
ISACCI(10,7)       MaxItSAC=N
ISACCI(10,8)       Selection/NoSelection                  --->   3/1

Dimension SACLMO(60)
SACLMO(1)          LMO/LMO=Boys/PM                        --->   2/1/2
SACLMO(2)          RightVecOnly
SACLMO(3)          EgOp/FullRGeneration                   --->   1/2
SACLMO(4)          LevelOne/LevelTwo/LevelThree           --->   1/2/3
SACLMO(5)          RefCIWind=(N, M)    for N
SACLMO(6)          RefCIWind=(N, M)    for M
SACLMO(7)          ScriptS
SACLMO(8)          ConvDiag=N
SACLMO(9)          ConvSAC=N
SACLMO(10)         ConvLin=N
```

SACLMO(11)	MaxItLin=N		
SACLMO(12)	Omega=val		
SACLMO(13)	CutOffDIIS=val		
SACLMO(14)	CutOffDIISZvec=val		
SACLMO(15)	TransitionFrom=SpinState= Singlet/Triplet/CationDoublet/AnionDoublet/ Quintet/Quartet/Sextet/Septet	--->	1/2/3/4/5/6/7/8
SACLMO(16)	TransitionFrom=Symmetry=N		
SACLMO(17)	TransitionFrom=Root=N		
SACLMO(18)	MaxEgOp=N		
SACLMO(19)	PrintOperator		
SACLMO(20)	PrintNaturalOrbital		
SACLMO(21)	PrintDensityMatrix		
SACLMO(22)	CThreEgABAOp=A1Op=val		
SACLMO(23)	CThreEgABAOp=A2Op=val		
SACLMO(24)	CThreEgAABAOp=A1Op=val		
SACLMO(25)	CThreEgAABAOp=A2Op=val		
SACLMO(26)	EgAOp=Type=S/SD	--->	1/2
SACLMO(27)	EgAOp=ActiveSpace=Small/Large	--->	2/1
SACLMO(28)	EgAOp=Selection/Noselection	--->	2/1
SACLMO(29)	EgBOp=Type=S/SD	--->	1/2
SACLMO(30)	EgBOp=ActiveSpace=Samll/Large	--->	2/1
SACLMO(31)	EgBOp=Selection/NoSelection	--->	2/1
SACLMO(32)	Ideriv (This is not a keyword)		
SACLMO(33)	CThreULS2G=val		
SACLMO(34)	CThreULS2E=val		
SACLMO(35)	CThreULR1=val		
SACLMO(36)	CThreULR2=val		
SACLMO(37)	CThreDensULS2=val		
SACLMO(38)	CThreDensULR1=val		
SACLMO(39)	RefCISD		
SACLMO(40)	Flag of keywords		
SACLMO(41)	WithoutDegeneracy		
SACLMO(42)	EThreDegFac		
SACLMO(43)	CThreDegULFac		
SACLMO(44)	not used		
SACLMO(45)	not used		
SACLMO(46)	not used		
SACLMO(47)	not used		
SACLMO(48)	not used		
SACLMO(49)	not used		
SACLMO(50)	not used		
SACLMO(51)	not used		
SACLMO(52)	not used		
SACLMO(53)	not used		
SACLMO(54)	not used		
SACLMO(55)	not used		
SACLMO(56)	not used		
SACLMO(57)	not used		

```
SACLMO(58)      not  used
SACLMO(59)      not  used
SACLMO(60)      not  used

Dimension SACFlg(5)
SACFlg(1)    mod(SACFlg/4**0,4**1)        Density
             mod(SACFlg/4**1,4**2)        NotransitionDensity
             mod(SACFlg/4**2,4**3)        SpinDensity
             mod(SACFlg/4**3,4**4)        Restart/Stop                  --->   1/2
             mod(SACFlg/4**4,4**5)        not  used
             mod(SACFlg/4**5,4**6)        Namelist
             mod(SACFlg/4**6,4**7)        not  used
             mod(SACFlg/4**7,4**8)        AddElectron/SubElectron       --->   1/2
             mod(SACFlg/4**8,4**9)        BGSUM/CGSUM/AGSUM             --->   1/2/3
             mod(SACFlg/4**9,4**10)       not  used
SACFlg(2)          AllProperties/NoProperty                  --->   1/2
SACFlg(3)          EThreEgR4
SACFlg(4)          MacroIter=N
SACFlg(5)          not used

Dimension SACThr(30,8)
             ===== Singlet State + Global =====
SACThr(  1,1)      SD-R/General-R                            --->   1/2
SACThr(  2,1)      Variational/NonVariational                --->   1/2
SACThr(  3,1)      InCoreDiag
SACThr(  4,1)      SelectionCISonly                          (Global)
SACThr(  5,1)      NoLinkedSelection
SACThr(  6,1)      NoUnLinkedSelection
SACThr(  7,1)      FullUnLinked
SACThr(  8,1)      WithoutR2S2                               (Global)
SACThr(  9,1)      MaxR=N
SACThr(10,1)       Iterative=non/Sinitial/SDInitial          --->   0/1/2
SACThr(11,1)       LinkedSelection/LinkedSelection=N         --->   0/1/2/3
SACThr(12,1)       CThreMainConfig=val                       (Global)
SACThr(13,1)       EThreS2=val                               (Global)
SACThr(14,1)       EThreR2=val
SACThr(15,1)       CThreEgULR=val
SACThr(16,1)       EThreEGR=val
SACThr(17,1)       PlusULG=ALL
SACThr(18,1)       PlusULG=S1S1
SACThr(19,1)       PlusULG=S1S2
SACThr(20,1)       PlusULG=S1S1S1
SACThr(21,1)       PlusULE=ALL
SACThr(22,1)       PlusULE=R1S1
SACThr(23,1)       PlusULE=R2S1
SACThr(24,1)       PlusULE=R2S2
SACThr(25,1)       CThreEgAB=B1Op=val
SACThr(26,1)       CThreEgAB=B2Op=val
SACThr(27,1)       CThreEgAAB=B1Op=val
```

```
SACThr(28,1)        CThreEgAAB=B2Op=val
SACThr(29,1)        not used
SACThr(30,1)        Density/TransitionDensity/NoTransitionDensity/SpinDensity
                                                        --->   1/2/4/16
              ===== Triplet State =====
SACThr(  1,2)       SD-R/General-R                      --->   1/2
SACThr(  2,2)       Variational/NonVariational          --->   1/2
SACThr(  3,2)       InCoreDiag
SACThr( 4,2)
SACThr(  5,2)       NoLinkedSelection
SACThr(  6,2)       NoUnLinkedSelection
SACThr(  7,2)       FullUnLinked
SACThr( 8,2)
SACThr(  9,2)       MaxR=N
SACThr(10,2)        Iterative=non/Sinitial/SDInitial    --->   0/1/2
SACThr(11,2)        LinkedSelection/LinkedSelection=N   --->   0/1/2/3
SACThr(12,2)
SACThr(13,2)
SACThr(14,2)        EThreR2=val
SACThr(15,2)        CThreEgULR=val
SACThr(16,2)        EThreEGR=val
SACThr(17,2)        PlusULG=ALL
SACThr(18,2)        PlusULG=S1S1
SACThr(19,2)        PlusULG=S1S2
SACThr(20,2)        PlusULG=S1S1S1
SACThr(21,2)        PlusULE=ALL
SACThr(22,2)        PlusULE=R1S1
SACThr(23,2)        PlusULE=R2S1
SACThr(24,2)        PlusULE=R2S2
SACThr(25,2)        CThreEgAB=B1Op=val
SACThr(26,2)        CThreEgAB=B2Op=val
SACThr(27,2)        CThreEgAAB=B1Op=val
SACThr(28,2)        CThreEgAAB=B2Op=val
SACThr(29,2)        not used
SACThr(30,2)        Density/TransitionDensity/NoTransitionDensity/SpinDensity
                                                        --->   1/2/4/16
              ===== CationDoublet State =====
SACThr( 1,3)--SACThr(30,3)
    All items are the same as those in triplet state
              ===== AnionDoublet State =====
SACThr( 1,3)--SACThr(30,4)
    All items are the same as those in triplet state
    Exception: SACThr(12,4) not used
              ===== Quartet State =====
SACThr( 1,4)--SACThr(30,5)
    All items are the same as those in triplet state
    Exception: SACThr(12,5) not used
              ===== Quintet State =====
SACThr( 1,6)--SACThr(30,6)
```

All items are the same as those in triplet state
Exception: SACThr(12,6) not used
===== Sextet State =====
SACThr(1,7)--SACThr(30,7)
All items are the same as those in triplet state
Exception: SACThr(12,7) not used
===== Septet State =====
SACThr(1,8)--SACThr(30,8)
All items are the same as those in triplet state
Exception: SACThr(12,8) not used

Dimension SACMth(8)

SACMth(1)	SD-*R*/General-*R*	--->	1/2	
SACMth(2)	SAConly	--->	1/2	(with Density)
SACMth(3)	SelectionOnly			
SACMth(4)	InCoreDiagSAC			
SACMth(5)	NonHF			
SACMth(6)	PrintMyIOp			
SACMth(7)	SkipSmallCI/SmallCI	--->	1/2	
SACMth(8)	not used			

IV-D. Remarks

(1) When SAC-CI keyword options are added, check ertgen.inc and make sure in size and modify the total size parameter, if necessary. Then, check common-array size in #ERuote# of L1.F.

(2) MacroIteration: L1.F is modified to make a route for carring out MacroIteration (see user's reference for details). The type of route for Macro-Iteration is 20 - 22. Therefore, the information is stored in JobDat(I,20) - JobDat(I,22) in #ERoute# of L1.F. Please find CompJT is alse modified for MacroIteration. Be careful on subroutine-argument for ISACMR in ERoute and CompJT, which is newly added.

Part V. Input and Output Examples

A. Input Examples

The input examples summarized in Table 1 are given below and in the directory g09/tests/com

Table 1. SAC/SAC-CI sample inputs

Input No	SD-*R* /G-*R*	Ene. /Opt.	NV /V	Diag.	Molecule	Level	CPU (sec) [b]	Comments
=== Instructive Inputs ===								
631	SD-*R*	Ene.	NV	Iter.	H_2O	N[a]	25s	Singlet, triplet, cation, anion, DZ basis, without selection, comparison with full-CI.
632	SD-*R*	Ene.	V	Iter.	H_2O	3	1m33s	Valence-Rydberg singlet & triplet excited states, ionized states compared with experiments.
633	SD-*R*	Ene.	V	Iter.	C_2H_4	3,2,1	2m13s	Introductory use of SAC-CI, Nature of the states and SAC-CI dimensions are examined beforehand using SelecCISonly, and then SAC-CI is executed.
634	SD-*R*	Ene.	V	Iter.	C_2H_4	3	9m1s	Singlet, triplet, ionized states are compared with exptl. values.
635	SD-*R*	Ene.	V	Iter.	C_2H_4	3,2,1	17m16s	Level1/Level2/Level3 are compared for singlet, triplet, ionized states.
636	SD-*R*	Ene.	V	Iter.	CO_2	3,2,1	28m32s	Singlet, triplet, ionized, electron-attached states Comparison of Level1/Level 2/Level3 and with exptl.
637	SD-*R*	Ene.	V	Iter.	Porphin	1	2h43m5s	Free Base Porphin; Q, B, N, L, M bands are calculated with 220 active space.
638	SD-*R*	Opt.	V	Iter.	HCF	3	20m31s	Geometry opt of ground A' and excited A'' states and adiabatic excitation energy.
639	SD-*R*	Opt.	V	Iter.	NH_2	3	1m24s	Open-shell opt; ground B_1, excited A_1 states are optimized and adiabatic ex. energy calculated.
640	SD-*R*	Ene.	V	Iter.	MoS_4^{2-}	2	35m24s	Transition metal complex, On/off of Without-Degeneracy option. Singlet

								excited states compared with exptl.
641	SD-*R*	Ene.	V	Iter.	Glyoxal	2	24m2s	Singlet, triplet, ionized states are calculated and compared with exptl.
642	SD-*R*	Ene.	V	Iter.	Acrolein	3	10m14s	LMO(Pipek-Mezey) for ground and singlet $n \rightarrow \Pi^*$ excited states, electron correlations are effectively calculated by using LMO.
643	SD-*R*	Ene.	NV	InCore	CH_2, CH^+	F [a]	19m47s	Full linked and unlinked terms within SD-*R*. Unimportance of the neglected terms. Equivalence of EOM-CC and CCLRT to SAC-CI.
644	SD-*R*	GSUM	V	InCore	Li_2	3	2m33s	GSUM: Potential energy curves of 5 singlet states are calculated by the GSUM method.
645	SD-*R*	Ene.	V	Iter.	N_2	N [a]	5m54s	High-spin states (quartet, quintet, sextet, septet), comparison with full-CI.
646	G-*R*	Ene.	V	Iter.	N_2	3	5m37s	Singet to septet states by general-*R* method: results are compared with full-CI.
647	G-*R*	Opt.	V	Iter.	BH	3	52s	General-*R* opt. Singlet Δ state (two-electron process; 2ep) is optimized by general-*R* method giving good agreement with experiment.
648	SD-*R*	Opt.	V	Iter.	C_2^+	3	11m3s	High-spin opt. Quartet Σ_g^- (2ep) and Σ_u^- (3ep) are optimized by DT-*R* and DTQ-*R*, the latter giving good agreement with experiment.
649	SD-*R*	Force	V	Iter.	HNO	3	1m50s	Force at vertical excited state; singlet A'', triplet A'', ionized A' states; force along internal coordinate.
650	SD-*R*	Ene.	V	Iter.	HCHO	3	12m58s	All properties (multipole moments, N-th moments, electrostatic properties, diamagnetic terms)
651	SD-*R*	Opt.	V	Iter.	HCHO	3	25m13s	Ground (C_{2v}), singlet A'', triplet A'' excited states (C_s) are optimized.
652	SD-*R*	Ene.	V	Iter.	CH_3, H_2O^+, NH_2	3	7s	ESR HFSC, open-shell radicals, full-active.
653	SD-*R*	Ene.	V	Iter.	Pyrrole	3	54m58s	Electron repulsion integr-

								als are separately allocated in memory and disk.
=== Inputs for detailed program check ===								
654	SD-*R*	Opt.	NV /V	Iter./ InCore	CO	3	13m14s	Comparison of four jobs, NV/V, Iter./InCore Singlet Σ^- state.
655	SD-*R*	Opt.	NV /V	Iter./ InCore	CO	3	13m53s	Comparison of four jobs, NV/V, Iter./InCore Triplet Π state.
656	SD-*R*	Opt.	NV /V	Iter./ InCore	CO	3	8m34s	Comparison of four jobs, NV/V, Iter./InCore Ionized Σ^+ state.
657	SD-*R*	Opt.	NV /V	Iter./ InCore	CO	3	8m46s	Comparison of four jobs, NV/V, Iter./InCore Ionized Σ^+ state Electron-attached Π state.
658	SD-*R*	Opt.	NV /V	Iter.	HCN	3	3m33s	Comparison of Canonical and MOD; NV/V, Can.(CMO)/ MOD(CMO), singlet A'' state.
659	SD-*R*	GSUM +Opt.	V	Iter.	HCN	3	5m53s	Combination of GSUM + Opt. Partial Opt. of H-C-N angle, singlet A' excited.
660	SD-*R*	Opt.	NV /V	Iter./ InCore	C_2^+	3	5m14s	Comparison of four jobs, NV/V, Iter./InCore Quartet Σ^- state SDTQ-*R*.
661	G-*R*	Opt.	V	Iter.	CH	3	45s	Open-shell, 2-nd doublet Σ^- state of CH by general-*R*.
662	G-*R*	Opt.	V	Iter.	BH	3	33s	Triplet Σ^- state of BH, test of SDT-*R* and SDTQ-*R*.
663	G-*R*	Opt.	V	Iter.	HCN	3	4m46s	Singlet A'' state (C_s) is optimized using LMO(PM) by general-*R*.
664	SD-*R*	Ene.	V	Iter.	C_2H_4	3	8s	Ionized states are calculated with CISD reference. 2ep is obtained by SD-*R*.
665	SD-*R*	Ene.	V	Iter.	H_2O	3	3s	Test of TransitionFrom, ionized, 2-nd state of A_1.
666	SD-*R*	Ene.	V	Iter.	H_2O	3	4s	Test of TransitionFrom, singlet, 2-nd state of A_1.
667	G-*R*	Ene.	V	Iter.	H_2O	3	1m29s	Satellite peaks, SDTQ-*R*, FullRGeneration.
668	G-*R*	Ene.	V	Iter.	H_2O	3	38s	Test of TransitionFrom, singlet, 2-nd state of A_1.
669	SD-*R*	Ene.	V	Iter.	CH_3	3	4s	CH_3^+ by SAC, CH_3 by electron-attachment of SAC-CI.
670	SD-*R*	Ene.	V	Iter.	CH_3	3	4s	CH_3^- by SAC, triplet state with ROHF MOs.

671	SD-*R*	Ene.	V	Iter.	CH_3	3	3s	CH_3^- by SAC, CH_3 by ionization of SAC-CI with ROHF MOs.
672	SD-*R*	Ene.	NV	Iter.	CH_3	3	3s	CH_3^- by SAC, CH_3 by ionization of SAC-CI with ROHF MOs.
673	G-*R*	Ene.	V	Iter.	H_2O	3	9s	H_2O^{++} by SAC, H_2O^+ by electron-attachment of SAC-CI with ROHF MOs of H_2O^+.
674	G-*R*	Ene.	V	Iter.	H_2O	3	7s	H_2O by SAC, H_2O^+ by ionization of SAC-CI with ROHF MOs of H_2O^+.
675	G-*R*	Ene.	V	Iter.	H_2O	3	7s	H_2O by SAC, H_2O^+ by ionization of SAC-CI with ROHF MOs of H_2O^+.
689	SD-*R*	GSUM +Opt.	V	Iter.	HCF	3	11m31s	Numerical requency calculation for the singlet A'' excited state of HCF.
921	SD-*R* direct	Ene.	V	Iter.	Porphin	3	3h 14m7s [c]	Free Base Porphin; Q, B, N, L, M bands are calculated with 220 active space.
922	SD-*R* direct	Opt.	V	Iter.	HCHO	3	5m25s [c]	Ground (C_{2v}), singlet A'', triplet A'' excited states (C_s) are optimized.
923	SD-*R* direct	Ene.	V	Iter.	Pyrrole	3	1h 1m27s [c]	Electron repulsion integrals are separately allocated in memory and disk.
924	SD-*R* direct	GSUM +Opt.	V	Iter.	HCF	3	16m10s [c]	Numerical requency calculation for the singlet A'' excited state of HCF.
925	SD-*R* Direct	Ene.	V	Iter.	R-methyloxirane	$\lambda_g=\lambda_e$ =1.0d-6	4h 41m47s	Rotatory strength of CD spectrum for singlet states of R-methyloxirane
965	SD-*R* direct	Ene.	V	Iter.	H_2O	3	25s [c]	O1s core ionized state of H_2O and N1s core ionized states of N_2
966	SD-*R* Direct	Ene.	V	Iter.	CO	3	1m0s [c]	C1s-π* and O1s-π* core excited states of CO

[a] N and F in Level column indicate No selection and No selection with Full-unlinked, respectively.
[b] CPU time is due to Compaq DS20E
[c] CPU time is due to Core 2 6700

B. Detailed Input Examples

SAC-CI input examples are given in $g09root/tests/com/test631.com-test675.com, test689.com, test921.com-test925.com, test965.com-test966.com. In this guide, test631, test635, test637, test 638, and test647 are shown.

Input 631

```
%mem=12mw
# SAC-CI(Singlet=(NState=(2,2,2,2),NonVariational),
          Triplet=(NState=(2,2,2,2),NonVariational),
          CationDoublet=(NState=(3,0,1,1),NonVariational),
          AnionDoublet=(NState=(2,0,1,2),NonVariational),
          FullActive,
          SD-R,
          NoLinkedSelection,
          NoUnLinkedSelection)
         /D95 Unit=Bohr Test
```

Gaussian Test Job 631:
SAC-CI SD-R NV calculations for singlet, triplet, ionized, and electron-attached states of H2O with Huzinaga-Dunning D95 basis. All the SCF MOs are included in the active space (FullActive) and SAC-CI calculations are performed without selections (NoLinkedSelection, NoUnLinkedSelection). The results are compared with the full-CI results calculated separately. See PartI-L of the SAC-CI Guide.
Reference: N. C. Handy, Chem. Phys. Lett. 74, 280 (1980); H. Nakatsuji, K. Hirao, Y. Mizukami, Chem. Phys. Lett. 179, 555 (1991).

```
   0   1
O      0.0              0.0              0.0
H      1.515263         0.0             -1.049898

H     -1.515263         0.0             -1.049898
```

Input 635

```
# SAC-CI(LevelOne,
          Singlet=(NState=(2,3,3,1,2,2,2,5)),
          Triplet=(NState=(2,3,3,1,2,2,2,5)),
          CationDoublet=(NState=(2,0,0,1,0,1,1,1)))
         /Gen Massage IOP(2/15=-1) test
```

Gaussian Test Job 635 (Part 1):
Comparison of LevelOne, LevelTwo, and LevelThree calculations for ethylene. First is LevelOne calculation.
SAC-CI SD-R calculations for singlet, triplet, and ionized states of ethylene using Huzinaga-Dunning basis with polarization functions [4s2p1d/2s1p] plus Rydberg functions [2s2p2d] on center of molecule. Inner-shells are excluded from the active space and full-valence active MOs are used (FC; default).
Dummy atom is used with symmetry (Massage,IOP(2/15=-1)).
The results are summarized in Part I-L of the SAC-CI Guide.

```
 0 1
H1
C2     1    r1
C3     2    r2    1    a1
H4     3    r1    2    a1    1      0.0
H5     3    r1    2    a1    1  180.0
H6     2    r1    3    a1    4  180.0
N7     2    r22  1    a1    4      0.0

r1=1.0868
r2=1.3391
a1=121.28
r22=0.66955

 C 0
 S     6    1.00
          4232.61000000              0.00202900
           634.88200000              0.01553500
           146.09700000              0.07541100
            42.49740000              0.25712100
            14.18920000              0.59655500
             1.96660000              0.24251700
 S     1    1.00
             5.14770000              1.00000000
 S     1    1.00
             0.49620000              1.00000000
 S     1    1.00
             0.15330000              1.00000000
 P     4    1.00
            18.15570000              0.01853400
             3.98640000              0.11544200
             1.14290000              0.38620600
             0.35940000              0.64008900
 P     1    1.00
             0.11460000              1.00000000
 D     1    1.00
             0.75000000              1.00000000
 ****
 H     0
 S     3    1.00
            19.24060000              0.03282800
             2.89920000              0.23120800
             0.65340000              0.81723800
 S     1    1.00
             0.17760000              1.00000000
 P     1    1.00
             1.00000000              1.00000000
 ****
```

```
 N     0
 S     1    1.00
              0.04370000              1.00000000
 S     1    1.00
              0.01725000              1.00000000
 P     1    1.00
              0.03990000              1.00000000
 P     1    1.00
              0.01575000              1.00000000
 D     1    1.00
              0.02850000              1.00000000
 D     1    1.00
              0.01125000              1.00000000
 ****

 7 Nuc 0.0

--Link1--
# SAC-CI(LevelTwo,
            Singlet=(NState=(2,3,3,1,2,2,2,5)),
            Triplet=(NState=(2,3,3,1,2,2,2,5)),
            CationDoublet=(NState=(2,0,0,1,0,1,1,1)))
          /Gen Massage IOP(2/15=-1) test

Gaussian Test Job 635 (Part 2):
SAC-CI SD-R LevelTwo calculations for ethylene.

 0 1
H1
C2     1    r1
C3     2    r2    1    a1
H4     3    r1    2    a1    1      0.0
H5     3    r1    2    a1    1  180.0
H6     2    r1    3    a1    4  180.0
N7     2    r22  1   a1    4      0.0

r1=1.0868
r2=1.3391
a1=121.28
r22=0.66955

 C 0
 S     6    1.00
         4232.61000000              0.00202900
           634.88200000              0.01553500
           146.09700000              0.07541100
            42.49740000              0.25712100
            14.18920000              0.59655500
             1.96660000              0.24251700
```

```
 S     1    1.00
              5.14770000          1.00000000
 S     1    1.00
              0.49620000          1.00000000
 S     1    1.00
              0.15330000          1.00000000
 P     4    1.00
             18.15570000          0.01853400
              3.98640000          0.11544200
              1.14290000          0.38620600
              0.35940000          0.64008900
 P     1    1.00
              0.11460000          1.00000000
 D     1    1.00
              0.75000000          1.00000000
 ****
 H     0
 S     3    1.00
             19.24060000          0.03282800
              2.89920000          0.23120800
              0.65340000          0.81723800
 S     1    1.00
              0.17760000          1.00000000
 P     1    1.00
              1.00000000          1.00000000
 ****
 N     0
 S     1    1.00
              0.04370000          1.00000000
 S     1    1.00
              0.01725000          1.00000000
 P     1    1.00
              0.03990000          1.00000000
 P     1    1.00
              0.01575000          1.00000000
 D     1    1.00
              0.02850000          1.00000000
 D     1    1.00
              0.01125000          1.00000000
 ****

 7 Nuc 0.0

--Link1--
# SAC-CI(LevelThree,
            Singlet=(NState=(2,3,3,1,2,2,2,5)),
            Triplet=(NState=(2,3,3,1,2,2,2,5)),
            CationDoublet=(NState=(2,0,0,1,0,1,1,1)))
          /Gen Massage IOP(2/15=-1) test
```

Gaussian Test Job 635 (Part 3):
SAC-CI SD-R LevelThree calculations for ethylene

```
 0 1
H1
C2     1    r1
C3     2    r2    1    a1
H4     3    r1    2    a1    1      0.0
H5     3    r1    2    a1    1  180.0
H6     2    r1    3    a1    4  180.0
N7     2    r22  1   a1    4      0.0

r1=1.0868
r2=1.3391
a1=121.28
r22=0.66955

 C 0
 S     6    1.00
          4232.61000000              0.00202900
           634.88200000              0.01553500
           146.09700000              0.07541100
            42.49740000              0.25712100
            14.18920000              0.59655500
             1.96660000              0.24251700
 S     1    1.00
             5.14770000              1.00000000
 S     1    1.00
             0.49620000              1.00000000
 S     1    1.00
             0.15330000              1.00000000
 P     4    1.00
            18.15570000              0.01853400
             3.98640000              0.11544200
             1.14290000              0.38620600
             0.35940000              0.64008900
 P     1    1.00
             0.11460000              1.00000000
 D     1    1.00
             0.75000000              1.00000000
 ****
 H     0
 S     3    1.00
            19.24060000              0.03282800
             2.89920000              0.23120800
             0.65340000              0.81723800
 S     1    1.00
             0.17760000              1.00000000
```

```
 P     1    1.00
            1.00000000              1.00000000
 ****
 N     0
 S     1    1.00
            0.04370000              1.00000000
 S     1    1.00
            0.01725000              1.00000000
 P     1    1.00
            0.03990000              1.00000000
 P     1    1.00
            0.01575000              1.00000000
 D     1    1.00
            0.02850000              1.00000000
 D     1    1.00
            0.01125000              1.00000000
 ****

 7 Nuc 0.0

### Input 637 ###

%mem=700MB
# SAC-CI(Singlet=(NState=(0,0,0,0,0,4,4,1)),
            LevelOne,Window=(25,244))/Gen Test

Gaussian Test Job 637:
SAC-CI SD-R LevelOne calculation of optically-allowed singlet excited
states of Free-Base Porphin using Huzinaga basis sets [4s2p/2s].
Inner-shells are excluded from the active space and full-valence
active MOs are used (FC; default): 57 occupied and 163 unoccupied
MOs are included in the active space of SAC-CI.
CPU memory of 700MB is specified with %mem to allocate electron
repulsion integrals in core memory (all ERIs are stored on cpu).
If the core memory is not enough for allocating all the repulsion
integrals, according to the available memory, the program will
automatically divide the integral file into appropriate number of
files which are sequentially allocated on the core memory.
Experimental results and the results of LevelTwo calculations are
compared in Part I-L of the SAC-CI Guide.

0 1
N        2.122283        0.000000        0.000000
C        2.903991        1.131654        0.000000
C        2.431060        2.448915        0.000000
C        1.087013        2.860819        0.000000
N        0.000000        2.032117        0.000000
C       -1.087013        2.860819        0.000000
C       -2.431060        2.448915        0.000000
```

C	-2.903991	1.131654	0.000000
N	-2.122283	0.000000	0.000000
C	-2.903991	-1.131654	0.000000
C	-2.431060	-2.448915	0.000000
C	-1.087013	-2.860819	0.000000
N	0.000000	-2.032117	0.000000
C	1.087013	-2.860819	0.000000
C	2.431060	-2.448915	0.000000
C	2.903991	-1.131654	0.000000
C	4.274858	-0.690194	0.000000
C	4.274858	0.690194	0.000000
H	5.131714	1.353489	0.000000
H	5.131714	-1.353489	0.000000
H	3.188699	-3.229008	0.000000
C	0.682348	-4.268828	0.000000
C	-0.682348	-4.268828	0.000000
H	-1.357121	-5.118337	0.000000
H	1.357121	-5.118337	0.000000
H	-3.188699	-3.229008	0.000000
C	-4.274858	-0.690194	0.000000
C	-4.274858	0.690194	0.000000
H	-5.131714	1.353489	0.000000
H	-5.131714	-1.353489	0.000000
H	-1.106269	0.000000	0.000000
H	-3.188699	3.229008	0.000000
C	-0.682348	4.268828	0.000000
C	0.682348	4.268828	0.000000
H	1.357121	5.118337	0.000000
H	-1.357121	5.118337	0.000000
H	3.188699	3.229008	0.000000
H	1.106269	0.000000	0.000000

```
C     0
S     5    1.00
          2659.7564          0.0021773
         398.69695           0.0166033
         90.755086           0.0802279
         25.636499           0.2577006
         8.2459146           0.4819621
S     1    1.00
         2.8051856           0.3122832
S     2    1.00
         5.1559447           -.0848345
         .47552582           0.5700241
S     1    1.00
         .14967892           0.5131541
P     4    1.00
         18.605948           0.0141713
         4.0986025           0.0878963
```

```
        1.1898171          0.2919946
        .38009675          0.5005517
P     1    1.00
        .12037644          0.3410139
****
N     0
S     5    1.00
        3664.0797          0.0021676
        545.49875          0.0166708
        123.85150          0.0807709
        35.000733          0.2598847
        11.305142          0.4827206
S     1    1.00
        3.8639685          0.3080344
S     2    1.00
        7.4487198          -.0839130
        .68502526          0.5690952
S     1    1.00
        .21183064          0.5153671
P     4    1.00
        26.573876          0.0147362
        5.9212438          0.0924189
        1.7325073          0.3000219
        .55217497          0.4983650
P     1    1.00
        .17185798          0.3351956
****
H     0
S     3    1.00
        19.2406            0.032828
        2.8992             0.231208
        0.6534             0.817238
S     1    1.00
        0.1776             1.000000
****

### Input 638 ###

%mem=12mw
# SAC-CI(Singlet=(NState=(0,1)),
            TargetState=(SpinState=Singlet,Symmetry=2,Root=1))
          /D95(d) Opt test

Gaussian Test Job 638 (Part 1):
SAC-CI SD-R geometry optimization for the singlet ground (A') and A"
excited state of HCF with D95(d) basis. Minimum-Orbital Deformation
(MOD) method is used and all the SCF MOs are included in the active
space. First is the geometry optimization for the excited A" state.
Initial geometry is the experimental one.
```

The results are compared with experiments in Part I-L of the
SAC-CI Guide.

```
0 1
C
F 1 FC
H 1 HC 2 HCF
Variables:
FC = 1.308
HC = 1.063
HCF = 123.8

--Link1--
%mem=12mw
# SAC-CI(SacOnly,
          TargetState=(SpinState=Singlet,Symmetry=1,Root=0))
         /D95(d) Opt test
```

Gaussian Test Job 638 (Part 2):
Geometry optimization of the SAC ground state of HCF.
Initial geometry is the experimental one. MacroIter=1 (default).

```
0 1
C
F 1 FC
H 1 HC 2 HCF
Variables:
FC = 1.305
HC = 1.138
HCF = 104.1
```

Input 647

```
%mem=12mw
# SAC-CI(Singlet=(NState=(0,1,0,0)),
          TargetState=(SpinState=Singlet,Symmetry=2,Root=1),
          General-R) /D95** Opt CPHF=Canonical test
```

Gaussian Test Job 647 (Part 1):
SAC-CI general-R geometry optimization calculation for the singlet
Delta excited state of BH with D95**. All the SCF MOs are included
in the active space (default of SAC-CI optimization). Initial
geometry is the experimental one. Since singlet delta excited
state is two-electron excited state, general-R method is more
reliable than the SD-R method. So, for comparison, SAC-CI SD-R
calculation is also done below for comparison. The results are
summarized in Part I-L of the SAC-CI Guide.

```
0 1
```

```
B
H 1 BH
Variables:
BH = 1.1963

--Link1--
%mem=12mw
# SAC-CI(Singlet=(NState=(0,1,0,0),MaxR=2),
            TargetState=(SpinState=Singlet,Symmetry=2,Root=1),
            General-R) /D95** Opt CPHF=Canonical test

Gaussian Test Job 647 (Part 2):
SAC-CI SD-R geometry optimization calculation for the singlet
Delta excited state of BH with full-active MOs of D95**.
Initial geometry is the experimental one.

0 1
B
H 1 BH
Variables:
BH = 1.1963

--Link1--
%mem=12mw
# SAC-CI(SacOnly,
            TargetState=(SpinState=Singlet,Symmetry=1,Root=0))
          /D95** Opt CPHF=Canonical test

Gaussian Test Job 647 (Part 3):
Geometry optimization calculation of the SAC ground state of BH
with full-active MOs of D95**.
Initial geometry is the experimental one.

0 1
B
H 1 BH
Variables:
BH = 1.232
```

C. Output Examples

SAC-CI output examples are given in $g09root/tests/sgi/test631.log -test675.log, test689.log, test921.log-test925.log, test965.log-test966.log. In this guide, test631, test635, test637, test 638, and test647 are shown. See section I-L for detailed description of the results.

Output 631

```
Entering Gaussian System, Link 0=/work/g03.C02/g03/g03
Initial command:
/work/g03.C02/g03/l1.exe /work/g03.C02/inputs/Gau-113419.inp -scrdir=/work/g03.C02/inputs/
Entering Link 1 = /work/g03.C02/g03/l1.exe PID=    113418.

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---------------------------------------------------------------
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M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
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K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,
A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

****************************************
Gaussian 03:  AI64T-G03RevC.02 12-Jun-2004
               31-Jul-2004
****************************************
%mem=12mw
-----------------------------------------------------------------------
# SAC-CI(Singlet=(NState=(2,2,2,2),NonVariational), Triplet=(NState=(2
,2,2,2),NonVariational), CationDoublet=(NState=(3,0,1,1),NonVariationa
l), AnionDoublet=(NState=(2,0,1,2),NonVariational), FullActive, SD-R,
NoLinkedSelection, NoUnLinkedSelection) /D95 Unit=Bohr Test
-----------------------------------------------------------------------
1/20=1,38=1/1;
2/17=6,18=5,40=1/2;
3/5=8,11=9,16=1,25=1,30=1,36=2/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=5,9=30000,10=90,40=1,42=2/1,4;
9//23;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;
-----------------------------------------------------------------------
Gaussian Test Job 631: SAC-CI SD-R NV calculations for singlet, triple
t, ionized, and electron-attached states of H2O with Huzinaga-Dunning
```

List of keywords given in the Gaussian input

Explanation of the test 631.

```
D95 basis. All the SCF MOs are included in the active space (FullActiv
e) and SAC-CI calculations are performed without selections (NoLinkedS
election, NoUnLinkedSelection). The results are compared with the full
-CI results calculated separately. See PartI-L of the SAC-CI Guide. Re
ference: N. C. Handy, Chem. Phys. Lett. 74, 280 (1980); H. Nakatsuji,
K. Hirao, Y. Mizukami, Chem. Phys. Lett. 179, 555 (1991).
---------------------------------------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
O                    0.        0.        0.
H                    1.51526   0.       -1.0499
H                   -1.51526   0.       -1.0499

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          8            0        0.000000    0.000000    0.000000
   2          1            0        0.801843    0.000000   -0.555582
   3          1            0       -0.801843    0.000000   -0.555582
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3
    1  O    0.000000
    2  H    0.975512   0.000000
    3  H    0.975512   1.603685   0.000000
Stoichiometry    H2O
Framework group  C2V[C2(O),SGV(H2)]
Deg. of freedom     2
Full point group                 C2V     NOp   4
Largest Abelian subgroup         C2V     NOp   4
Largest concise Abelian subgroup C2      NOp   2
                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          8            0        0.000000    0.000000    0.111116
   2          1            0        0.000000    0.801843   -0.444466
   3          1            0        0.000000   -0.801843   -0.444466
---------------------------------------------------------------------
Rotational constants (GHZ):    914.6416683    389.9633196    273.3982351
Standard basis: D95 (6D, 7F)
There are     8 symmetry adapted basis functions of A1  symmetry.
There are     0 symmetry adapted basis functions of A2  symmetry.
There are     2 symmetry adapted basis functions of B1  symmetry.
There are     4 symmetry adapted basis functions of B2  symmetry.
Integral buffers will be    131072 words long.
```

Nuclear coordinates for H_2O given in the Gaussian input

Nuclear coordinates used in the actual calculation

```
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   14 basis functions,    32 primitive gaussians,    14 cartesian basis functions
    5 alpha electrons        5 beta electrons
      nuclear repulsion energy         9.0093542297 Hartrees.
NAtoms=    3 NActive=    3 NUniq=    2 SFac= 2.76D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    14 RedAO= T  NBF=     8     0     2     4
NBsUse=    14 1.00D-06 NBFU=     8     0     2     4
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.78D-01 ExpMax= 7.82D+03 ExpMxC= 1.18D+03 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=         1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Initial guess orbital symmetries:
      Occupied  (A1) (A1) (B2) (A1) (B1)
      Virtual   (A1) (B2) (B1) (A1) (B2) (A1) (B2) (A1) (A1)
The electronic state of the initial guess is 1-A1.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=      826205.
SCF Done:  E(RHF) =  -76.0098376028     A.U. after   11 cycles
            Convg  =    0.5275D-09             -V/T =  2.0004
            S**2   =   0.0000
Range of M.O.s used for correlation:     1    14
NBasis=    14 NAE=     5 NBE=     5 NFC=     0 NFV=     0
NROrb=     14 NOA=     5 NOB=     5 NVA=     9 NVB=     9
--------------------------------------------------------------------
####################################################################
--------------------------------------------------------------------
              SAC/SAC-CI Program Combined with GAUSSIAN
                          for Calculating
        Ground, Excited, Ionized, and Electron-Attached States
                              and
            Singlet, Doublet, Triplet, Quartet, Quintet,
                  Sextet, and Septet Spin States
                              and
                 Their Analytical Energy Gradients
                        coded originally by
                         Hiroshi Nakatsuji
                          and extended by
 H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa,
       M. Ishida, T. Nakajima, Y. Honda, O. Kitao, and H. Nakai
                              at
                 Department of Hydrocarbon Chemistry,
                Division of Molecular Engineering, and
      Department of Synthetic Chemistry & Biological Chemistry,
                 Graduate School of Engineering,
```

Hartree-Fock SCF energy.

AO to MO transformation of two-electron repulsion integrals

Beginning of the SAC-CI part of the program (Link 923)

```
                         Kyoto University,
                       Kyoto 606-8501, Japan
-------------------------------------------------------------------------
#########################################################################
-------------------------------------------------------------------------
No. of INTEGRALS =      1925 NBLK =         1 KOUNT =       325
#############################################################################
    Singles-Doubles (SD) SAC/SAC-CI  (SAC-CI SD-R)
#############################################################################
================================================================
  STEP #PRES#  Generation of Linked Operators and Selection
================================================================
== States to be calculated ==
           A1   A2   B1   B2
SINGLET    Yes  Yes  Yes  Yes
TRIPLET    Yes  Yes  Yes  Yes
IONIZED    Yes  Yes  Yes  Yes
ANIONIZED  Yes  Yes  Yes  Yes
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  3,  2,  2,  2)
 Main reference configuration (CThreMainConfig) =  0.100D+00 (ISEL=2)
 Threshold for perturbation selection of linked operator
  EThreS2 (Lambda_G)=  0.000D+00(au)   EThreR2 (Lambda_E)=  0.000D+00(au)
TRIPLET STATE
 Number of States  Triplet      =(  2,  2,  2,  2)
 Main reference configuration (CThreMainConfig) =  0.100D+00 (ISEL=2)
 Threshold for perturbation selection of linked operator
  EThreR2 (Lambda_E)=  0.000D+00(au)
IONIZED STATE
 Number of States  CationDoublet=(  3,  0,  1,  1)
 Main reference configuration (CThreMainConfig) =  0.100D+00 (ISEL=2)
 Threshold for perturbation selection of linked operator
  EThreR2 (Lambda_E)=  0.000D+00(au)
ANION STATE
 Number of States  AnionDoublet =(  2,  0,  1,  2)
 Main reference configuration (CThreMainConfig) =  0.100D+00 (ISEL=2)
 Threshold for perturbation selection of linked operator
  EThreR2 (Lambda_E)=  0.000D+00(au)
****************************
        SINGLET STATE
****************************
-------------------------------------------------------------
LINKED OPERATORS FOR SAC:    SYMMETRY = A1  GROUND STATE
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            19         341          360
    AFTER             19         341          361
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = A1  EXCITED STATE
```

Description of the SAC/SAC-CI calculations. States to be calculated, Number of solution in each spin- and space-symmetry, thresholds for the perturbation selection.

Number of the linked operators for single- and double- excitation in the SAC w.f. before and after the perturbation selection

```
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.427495
       4 ->   6     0.98718
    ##   2-nd state ##       energy (au) =       0.704079
       3 ->   7     0.93996        5 ->   8    -0.27513
       4 ->   9    -0.16299
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            19         341          360
    AFTER             19         341          361
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = A2  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.418106
       5 ->   7     0.98426        5 ->  12    -0.16618
    ##   2-nd state ##       energy (au) =       1.010143
       5 ->  10     0.97923        5 ->  12    -0.18078
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             4         188          192
    AFTER              4         188          192
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.351624
       5 ->   6     0.99012
    ##   2-nd state ##       energy (au) =       0.895104
       5 ->   9     0.97846        5 ->  11    -0.12546
       4 ->   8    -0.12495        5 ->   6    -0.10331
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             8         208          216
    AFTER              8         208          216
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.505490
       4 ->   7     0.97419        3 ->   6    -0.15723
       4 ->  12    -0.13063
    ##   2-nd state ##       energy (au) =       0.589118
       3 ->   6     0.97967        4 ->   7     0.15663
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            14         298          312
    AFTER             14         298          312
****************************
        TRIPLET STATE
****************************
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = A1  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.369139
       4 ->   6     0.97263        3 ->   7     0.14860
```

Main configurations of the reference SECI calculation used for the perturbation selection step. For example, the first excited state in singlet A_1 symmetry is the transition from 4-th MO to 6-th MO, and its CI coefficient is about 0.99.

Main configurations of the reference SECI calculation used for the perturbation selection step. For example, the first excited state in triplet A_1 symmetry is the transition from 4-th MO to 6-th MO, and its CI coefficient is about 0.97.

```
      4 ->  11    -0.11461
   ##   2-nd state ##       energy (au) =       0.573102
      3 ->   7     0.94603        3 ->  12    -0.19765
      4 ->   6    -0.16874        2 ->   6    -0.12750
      5 ->   8     0.10952
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            19         398          417
    AFTER             19         398          417
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = A2  EXCITED STATE
  #SECI# Main reference configuration and coefficient
   ##   1-st state ##       energy (au) =       0.393888
      5 ->   7     0.97942        5 ->  12    -0.18897
   ##   2-nd state ##       energy (au) =       0.986890
      5 ->  10     0.96293        5 ->  12    -0.20176
      3 ->   8     0.14213        5 ->   7    -0.10891
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             4         270          274
    AFTER              4         270          274
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1  EXCITED STATE
  #SECI# Main reference configuration and coefficient
   ##   1-st state ##       energy (au) =       0.312730
      5 ->   6     0.98522        5 ->  11    -0.11693
   ##   2-nd state ##       energy (au) =       0.848620
      5 ->   9     0.85870        4 ->   8     0.49123
      5 ->  11    -0.10337
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             8         286          294
    AFTER              8         286          294
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2  EXCITED STATE
  #SECI# Main reference configuration and coefficient
   ##   1-st state ##       energy (au) =       0.432897
      4 ->   7     0.91078        3 ->   6     0.36043
      4 ->  12    -0.17578
   ##   2-nd state ##       energy (au) =       0.513023
      3 ->   6     0.91072        4 ->   7    -0.36545
      3 ->  11    -0.12102
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            14         396          410
    AFTER             14         396          410
****************************
        IONIZED STATE
****************************
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = A1  EXCITED STATE
  #SECI# Main reference configuration and coefficient
   ##   1-st state ##       energy (au) =       0.552964
```

Main configurations of the reference SECI calculation used for the perturbation selection step. The first ionized (cation doublet) state in A_1 symmetry is the ionization from 4-th MO, and its CI coefficient is about 1.00.

```
      4     1.00000
    ##   2-nd state ##       energy (au) =       1.345949
      2     1.00000
    ##   3-th state ##       energy (au) =      20.558147
      1     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             3          79          82
    AFTER              3          79          82
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.502475
      5     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1          47          48
    AFTER              1          47          48
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.717230
      3     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1          65          66
    AFTER              1          65          66
****************************
   ELECTRON ATTACHED STATE
****************************
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = A1  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.214035
      6     1.00000
    ##   2-nd state ##       energy (au) =       0.891793
      9     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             5         145         150
    AFTER              5         145         150
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.867550
      8     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1          71          72
    AFTER              1          71          72
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.306149
```

Main configurations of the reference SECI calculation used in the perturbation selection step. The first state in electron-attached (anion doublet) A_1 symmetry is the electron-attachment to 6-th MO, and its CI coefficient is about 1.00.

```
       7     1.00000
    ##   2-nd state ##       energy (au) =       0.943265
      10     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             3         131          134
    AFTER              3         131          134
================================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A1    CONVERGED
Solution for Singlet   A1    CONVERGED
Solution for Singlet   A2    CONVERGED
Solution for Singlet   B1    CONVERGED
Solution for Singlet   B2    CONVERGED
================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
================================================================
Threshold for S2 operator (CThreULS2G) 0.000D+00
================================================================
  STEP #SAC#  Solution of SAC equation
================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-05
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Solution for SAC equation converged
*******************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*******************************************
HF ENERGY     =     -76.009838 (AU)
SAC-NV  ENERGY=      -0.146417 (AU)
TOTAL ENERGY  =     -76.156254 (AU)
SAC-NV  coefficients (|C|>=0.03)
*SINGLE EXCITATION
*DOUBLE EXCITATION
       5    8    4    9     -0.07153         3   12    3    7      0.06227
       5    8    5    8     -0.05754         5    8    3    7     -0.05417
       4    9    3    7     -0.05004         4    9    4    9     -0.04729
       5    8    3   12      0.04450         5    8    2    6      0.04406
       3    7    3    7     -0.04338         5    8    2   13     -0.04316
       4    6    3    7     -0.04263         4    9    3   12      0.04046
       3    7    2    6      0.03683         4    9    2   13     -0.03628
       3   12    3   12     -0.03501         3   11    3    6      0.03462
```

Result of SAC calculation. Hartree-Fock (HF) energy, SAC-NV energy (correlation energy obtained with the SAC method), and the SAC-NV coefficients are shown. HF configuration always has 1.00 in the SAC wave function.

```
      5    8    3   10     -0.03383        4    9    2    6      0.03322
      4    6    2    6      0.03283        4    7    3    6     -0.03277
      3   12    2   11      0.03152        4   12    3   11     -0.03116
      4   11    3   12     -0.03004
Hartree-Fock configuration   1.00000
=================================================================
  STEP #ULINTS#  Unlinked integral for Singlet Excited State (SAC-CI)
=================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.000D+00 0.000D+00
Threshold for S2 operators (CThreULS2) 0.000D+00
==============================================================
  STEP #SCINV#  Iterative Diagonalization of SAC-CI-NV
==============================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
-- Right vectors --
Solution for   1-th A1     CONVERGED
Solution for   2-th A1     CONVERGED
Solution for   3-th A1     CONVERGED
-- Left vectors --
Solution for   1-th A1     CONVERGED
Solution for   2-th A1     CONVERGED
Solution for   3-th A1     CONVERGED
-- Right vectors --
Solution for   1-th A2     CONVERGED
Solution for   2-th A2     CONVERGED
-- Left vectors --
Solution for   1-th A2     CONVERGED
Solution for   2-th A2     CONVERGED
-- Right vectors --
Solution for   1-th B1     CONVERGED
Solution for   2-th B1     CONVERGED
-- Left vectors --
Solution for   1-th B1     CONVERGED
Solution for   2-th B1     CONVERGED
-- Right vectors --
Solution for   1-th B2     CONVERGED
Solution for   2-th B2     CONVERGED
-- Left vectors --
Solution for   1-th B2     CONVERGED
Solution for   2-th B2     CONVERGED
***********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
***********************************************
*******************************************************
Singlet       A1      ******************************************************
###   1-st  ###           ---   3rd state in this spin multiplicity ---
    Total energy       in au =     -75.761035
    Correlation energy in au =       0.248803
```

Result of SAC-CI calculation. Total energy, correlation energy (HF energy as the reference), excitation energy (SAC total energy as the reference), and the SAC-CI coefficients are shown. For example, the first excited state in singlet A_1 symmetry is the excitation from 4-th MO to 6-th MO, and its coefficient is 0.97. The excitation energy is 10.75 eV.

```
    Excitation energy  in au =       0.395220    in eV =      10.754473
  *SINGLE EXCITATION
       4    6     0.96936         3    7    -0.06892
       5    8    -0.05318         4   11    -0.04929
       2    6     0.04345         4   13    -0.03264
  *DOUBLE EXCITATION
       4    6    3    7    -0.12164         4    9    4    6    -0.11048
       4    7    3    6    -0.08080         4    6    4    6    -0.07322
       4    6    3   12     0.07235         5    8    4    6    -0.06335
       4    7    4    7    -0.04726         4    6    2    6     0.04284
       4   12    4    7     0.03945         4    7    3   11     0.03706
       3    7    2    6    -0.03486         4   11    4    6     0.03408
       4    9    2    6    -0.03402         3   12    2    6     0.03322
###   2-nd  ###           ---   6th state in this spin multiplicity ---
    Total energy       in au =     -75.454280
    Correlation energy in au =       0.555558
    Excitation energy  in au =       0.701974    in eV =      19.101697
  *SINGLE EXCITATION
       3    7    -0.94512         5    8     0.20556
       4    9     0.14298         4    6    -0.05098
       3   12     0.03793         4   11    -0.03185
  *DOUBLE EXCITATION
       3    6    3    6     0.08281         3    7    3    7     0.08003
       3   11    3    6    -0.06184         4    6    3    7     0.05638
       4    7    3    6     0.05435         4    7    2    7     0.05380
       4    9    3    7     0.04293         3    7    2    6    -0.04225
       4   12    2    7    -0.03856         5    7    5    7     0.03828
       3   12    3   10     0.03625         5    8    3   12     0.03565
       5    8    3    7     0.03367         3   11    2    7    -0.03301
       4   12    3    6    -0.03128         5   12    5    7    -0.03068
*******************************************************************************
Singlet       A2      ******************************************************
###   1-st  ###           ---   2nd state in this spin multiplicity ---
    Total energy       in au =     -75.761966
    Correlation energy in au =       0.247871
    Excitation energy  in au =       0.394288    in eV =      10.729122
  *SINGLE EXCITATION
       5    7     0.97160         5   12    -0.10814
  *DOUBLE EXCITATION
       5    7    3    7    -0.14357         5    8    5    7    -0.09639
       5    7    4    6    -0.07738         5    6    3    6    -0.07279
       5    7    3   12     0.06903         5    7    4    9    -0.06888
       5    6    4    7    -0.06754         5    7    2    6     0.06479
       5    6    2    7     0.04948         5    6    3   11     0.04229
       5    7    2   11    -0.03745         5   11    2    7    -0.03356
       5    7    4   11     0.03309
###   2-nd  ###           ---   8th state in this spin multiplicity ---
    Total energy       in au =     -75.181503
    Correlation energy in au =       0.828334
```

```
    Excitation energy  in au =       0.974751    in eV =      26.524322
  *SINGLE EXCITATION
       5   10    -0.95512         5   12     0.07695
  *DOUBLE EXCITATION
       5    7    4    6    -0.12591         5   10    5    8     0.12347
       5    6    4    7     0.10683         5   10    4    9     0.07674
       5   10    2    6    -0.05741         5   10    3   10     0.05595
       5    8    5    7    -0.05373         5   12    4    6     0.05190
       5   10    3   12    -0.05105         5    7    3    7    -0.05014
       5   10    3    7     0.04991         5   12    3    7     0.04832
       5    9    4    7    -0.04404         5    7    4    9    -0.04235
       5    6    2   10    -0.04144         5    9    4   10     0.04004
       5   12    3   12    -0.03940         5   11    2   10     0.03304
       5   10    2   13     0.03224         5    9    3    6    -0.03200
       5   10    2   11     0.03143         5    7    3   12     0.03057
       5   11    3   11    -0.03037
*****************************************************************************
Singlet       B1      ******************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    Total energy       in au =     -75.840435
    Correlation energy in au =       0.169403
    Excitation energy  in au =       0.315819    in eV =       8.593881
  *SINGLE EXCITATION
       5    6     0.97349         5   11    -0.05806
       5    9     0.04539         5   13    -0.03025
  *DOUBLE EXCITATION
       5    6    3    7    -0.12645         5    8    5    6    -0.10486
       5    6    2    6     0.09802         5    7    3    6    -0.09164
       5    6    3   12     0.08051         5    6    4    9    -0.07906
       5    6    4    6    -0.07158         5    7    4    7    -0.04967
       5    7    3   11     0.03878         5   12    3    6     0.03634
       5    6    2   11    -0.03564         5    6    2   13    -0.03175
###   2-nd  ###           ---   7th state in this spin multiplicity ---
    Total energy       in au =     -75.238252
    Correlation energy in au =       0.771585
    Excitation energy  in au =       0.918002    in eV =      24.980111
  *SINGLE EXCITATION
       5    9    -0.98251         5   11     0.10213
       4    8     0.04720         5    6     0.03546
  *DOUBLE EXCITATION
       5    8    5    6    -0.08035         5    9    5    8     0.06907
       5    9    4    9     0.05643         5    6    4    9    -0.04957
       5    6    3   10    -0.04677         5    6    2    6     0.04290
       5    9    2    6    -0.03541         5    9    3    7     0.03500
       5   10    4    7    -0.03396         5   10    3    6    -0.03351
       5    9    4    6    -0.03346
*****************************************************************************
Singlet       B2      ******************************************************
###   1-st  ###           ---   4th state in this spin multiplicity ---
```

```
    Total energy       in au =     -75.670341
    Correlation energy in au =       0.339497
    Excitation energy  in au =       0.485914    in eV =      13.222386
  *SINGLE EXCITATION
       4    7    -0.96291         3    6     0.12904
       4   12     0.08018

     4   10    -0.03911
       3   11    -0.03904
  *DOUBLE EXCITATION
       4    7    4    6     0.14773         4    7    3    7     0.12427
       4    9    4    7     0.09933         4    6    3    6     0.07498
       5    8    4    7     0.05488         4    7    3   12    -0.05286
       4   11    4    7    -0.05038         4    7    2    6    -0.04955
       3    7    2    7     0.04719         4    6    3   11    -0.04501
       3    7    3    6    -0.03851         3   11    3    7     0.03444
       3   12    2    7    -0.03387         4   12    4    6    -0.03043
###   2-nd  ###           ---   5th state in this spin multiplicity ---
    Total energy       in au =     -75.568589
    Correlation energy in au =       0.441248
    Excitation energy  in au =       0.587665    in eV =      15.991177
  *SINGLE EXCITATION
       3    6     0.97067         4    7     0.12820
       3    9     0.05352         4   10     0.03515
  *DOUBLE EXCITATION
       3    7    3    6    -0.15790         4    7    3    7    -0.08071
       3   10    3    6    -0.05351         4    9    3    6    -0.05351
       5    8    3    6    -0.04827         3   11    2    6     0.04380
       3   12    3    6     0.04330         4   12    2    6     0.04067
       4    7    4    6    -0.03197         3   11    3    7     0.03193
       4    7    2    6    -0.03122
=================================================================
  STEP #DENS#  Density Calculation
=================================================================
Transition density for SAC/SAC-CI (NV)
Threshold for S2 operators (CThreDensULS2):  0.00D+00
Threshold for R1,R2 operators (CThreDensULR1):  0.00D+00
Only right vectors are used. (ILEFT=0)
-------------------------------------------------------------------------
Transition dipole moment of   singlet state from SAC ground state
-------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
-------------------------------------------------------------------------
   A1         0      0.0          Excitations are from this state.
   A1         1     10.7545      0.0000      0.0000      0.6593      0.1145
   A1         2     19.1017      0.0000      0.0000     -0.7882      0.2907
   A2         1     10.7291      0.0000      0.0000      0.0000      0.0000
   A2         2     26.5243      0.0000      0.0000      0.0000      0.0000
```

Transition dipole moments and oscillator strengths of the excited states.are summarized. SAC w.f. is used for the ground state.

```
   B1          1       8.5939       0.2738       0.0000       0.0000       0.0158
   B1          2      24.9801       0.0961       0.0000       0.0000       0.0056
   B2          1      13.2224       0.0000      -0.6270       0.0000       0.1273
   B2          2      15.9912       0.0000       1.1672       0.0000       0.5337
-------------------------------------------------------------------------------
=================================================================
  STEP #CIMX#  CI matrix elements          ### TRIPLET STATE ###
=================================================================
=================================================================
  STEP #DIAGCI#  Solution of SDCI
=================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Triplet   A1    CONVERGED
Solution for Triplet   A2    CONVERGED
Solution for Triplet   B1    CONVERGED
Solution for Triplet   B2    CONVERGED
=================================================================
  STEP #ULINTT#  Unlinked integral for Triplet State (SAC-CI)
=================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.000D+00 0.000D+00
Threshold for S2 operators (CThreULS2) 0.000D+00
=================================================================
  STEP #SCINV#  Iterative Diagonalization of SAC-CI-NV
=================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
-- Right vectors --
Solution for   1-th A1     CONVERGED
Solution for   2-th A1     CONVERGED
-- Left vectors --
Solution for   1-th A1     CONVERGED
Solution for   2-th A1     CONVERGED
-- Right vectors --
Solution for   1-th A2     CONVERGED
Solution for   2-th A2     CONVERGED
-- Left vectors --
Solution for   1-th A2     CONVERGED
Solution for   2-th A2     CONVERGED
-- Right vectors --
Solution for   1-th B1     CONVERGED
Solution for   2-th B1     CONVERGED
-- Left vectors --
Solution for   1-th B1     CONVERGED
Solution for   2-th B1     CONVERGED
-- Right vectors --
Solution for   1-th B2     CONVERGED
Solution for   2-th B2     CONVERGED
-- Left vectors --
```

```
Solution for   1-th B2     CONVERGED
Solution for   2-th B2     CONVERGED
*********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
*********************************************
*****************************************************
Triplet       A1      ****************************
###   1-st  ###           ---   2nd state in this sp
    Total energy       in au =     -75.799083
    Correlation energy in au =       0.210754
    Excitation energy  in au =       0.357171    in eV =       9.719116
  *SINGLE EXCITATION
       4    6    -0.97197         3    7    -0.09965
       4   11     0.08592         4    9    -0.04541
       4   13     0.04474         2    6     0.03052
  *DOUBLE EXCITATION
       4    9    4    6     0.10516         5    8    4    6     0.06520
       3    7    4    6     0.06509         3   12    4    6    -0.05764
       4    6    3    7    -0.05568         2   13    4    6     0.03778
       4   11    4    6    -0.03528         4    7    3    6    -0.03244
       3   11    4    7    -0.03064
###   2-nd  ###           ---   6th state in this spin multiplicity ---
    Total energy       in au =     -75.568723
    Correlation energy in au =       0.441115
    Excitation energy  in au =       0.587532    in eV =      15.987548
  *SINGLE EXCITATION
       3    7    -0.94948         3   12     0.17321
       2    6     0.12988         5    8    -0.10474
       4    6     0.10261         4    9    -0.06893
       2   11    -0.03985         3   10    -0.03758
  *DOUBLE EXCITATION
       4    7    3    6     0.08515         4    6    3    7     0.06875
       3   10    3    7     0.05183         4    9    3    7     0.03990
       3    6    2    7     0.03825         3   12    3    7    -0.03785
       3   11    2    7    -0.03429         5    8    3   12     0.03382
       4   12    3    6    -0.03251         5    8    3    7     0.03132
       4    9    3   12     0.03066
*************************************************************************
Triplet       A2      ****************************************************
###   1-st  ###           ---   3rd state in this spin multiplicity ---
    Total energy       in au =     -75.780262
    Correlation energy in au =       0.229575
    Excitation energy  in au =       0.375992    in eV =      10.231266
  *SINGLE EXCITATION
       5    7    -0.97117         5   12     0.13391
       5   10    -0.03690
  *DOUBLE EXCITATION
       5    8    5    7     0.10633         5    7    4    6    -0.08505
       5    6    3    6    -0.08110         5    7    3    7    -0.08093
```

Result of SAC-CI calculation for triplet state. Total energy, correlation energy (HF energy as the reference), excitation energy (SAC total energy as the reference), and the SAC-CI coefficients are shown. For example, the first excited state in triplet A_1 symmetry is the triplet excitation from 4-th MO to 6-th MO, and its coefficient is -0.97. The excitation energy is 9.72 eV.

```
      3   12    5    7    -0.07743         5    6    4    7    -0.07569
      5    7    2    6     0.06702         4    9    5    7     0.06684
      2    7    5    6     0.05216         5   12    3    7    -0.03499
      2   11    5    7     0.03462         2   13    5    7     0.03443
      3   10    5    7     0.03211
###   2-nd  ###           ---   8th state in this spin multiplicity ---
   Total energy       in au =     -75.197414
   Correlation energy in au =       0.812423
   Excitation energy  in au =       0.958840    in eV =      26.091362
  *SINGLE EXCITATION
      5   10    -0.71791         5   12     0.09881
      3    8    -0.06479         5    7     0.04164
  *DOUBLE EXCITATION
      5    6    3    6    -0.43255         5    7    3    7     0.33090
      5    6    4    7    -0.31909         4    7    5    6    -0.16815
      5    7    4    6     0.16236         5    7    3   12    -0.13095
      5   12    3    7    -0.11049         5    7    4    9     0.10772
      5    6    4   12     0.09919         5    7    4   11    -0.09322
      5   10    5    8    -0.07839         5    6    3   11     0.07482
      5   10    4    9    -0.05671         4   10    5    6    -0.05621
      3   10    5    7    -0.05544         5   11    3    6     0.05313
      5   10    2    6     0.04944         5    6    3   13     0.04772
      4   10    5    9    -0.04740         5   13    3    6     0.04493
      5    7    2    6    -0.04388         2   10    5    6     0.04324
      5   12    3   12     0.04264         5    9    4    7     0.04186
      5    6    4   10    -0.03980         5   12    4    6    -0.03899
      4   12    5    6     0.03865         5    9    4   10    -0.03831
      3   12    5   10    -0.03815         5   10    3   10    -0.03415
      4   11    5    7    -0.03394         5    7    2   11     0.03350
*****************************************************************************
Triplet       B1      ***********************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
   Total energy       in au =     -75.869964
   Correlation energy in au =       0.139874
   Excitation energy  in au =       0.286291    in eV =       7.790371
  *SINGLE EXCITATION
      5    6    -0.97408         5   11     0.08488
      5   13     0.05439         5    9    -0.05139
      2    8     0.03137
  *DOUBLE EXCITATION
      5    8    5    6     0.11379         4    9    5    6     0.07519
      3    7    5    6     0.06930         3   12    5    6    -0.06666
      5    6    3    7    -0.06100         5    6    4    6    -0.05711
      5    7    4    7    -0.05444         2   13    5    6     0.03910
      2   11    5    6     0.03789         5   11    2    6     0.03522
###   2-nd  ###           ---   7th state in this spin multiplicity ---
   Total energy       in au =     -75.283029
   Correlation energy in au =       0.726809
   Excitation energy  in au =       0.873226    in eV =      23.761683
```

```
  *SINGLE EXCITATION
      5    9    -0.91683         4    8    -0.35605
      5   11     0.09665         5    6     0.04157
      5   13    -0.03089         2    8    -0.03036
  *DOUBLE EXCITATION
      5    9    5    8    -0.07542         3    9    5    7    -0.04814
      2    9    5    6     0.04431         5   11    2    9     0.03949
      5    6    2    6    -0.03652         5    9    2    6     0.03617
      5   12    3    9    -0.03418         4    9    5    6    -0.03390
      5   10    4    7     0.03339         5    7    4   10     0.03282
      5    9    3    7    -0.03248         3   12    5    9    -0.03226
*****************************************************************************
Triplet       B2      ******************************************************
###   1-st  ###           ---   4th state in this spin multiplicity ---
    Total energy       in au =     -75.722134
    Correlation energy in au =       0.287703
    Excitation energy  in au =       0.434120    in eV =      11.813011
  *SINGLE EXCITATION
      4    7     0.94571         3    6     0.24010
      4   12    -0.13599         3   11    -0.04416
  *DOUBLE EXCITATION
      4    9    4    7    -0.09520         4    7    3    7     0.06949
      3   12    4    7     0.06944         4    6    3    6     0.06657
      5    8    4    7    -0.05650         4    7    2    6    -0.04848
      4    6    2    7    -0.03479         2    7    4    6    -0.03292
      3    7    3    6    -0.03165         2   13    4    7    -0.03081
      4   12    3    7     0.03060         5    8    4   12    -0.03020
###   2-nd  ###           ---   5th state in this spin multiplicity ---
    Total energy       in au =     -75.634992
    Correlation energy in au =       0.374846
    Excitation energy  in au =       0.521263    in eV =      14.184284
  *SINGLE EXCITATION
      3    6    -0.94546         4    7     0.23570
      3   11     0.10887         2    7     0.08693
      3    9    -0.05096         3   13     0.04611
      2   12    -0.04080
  *DOUBLE EXCITATION
      4    7    3    7     0.07655         4    6    3    6     0.06576
      4    9    3    6     0.05616         5    8    3    6     0.04769
      4   12    2    6    -0.03730         3   10    3    6     0.03695
      3   11    3    7    -0.03639         3    6    2    6     0.03500
      2   13    3    6     0.03426         3    7    3    6     0.03307
=================================================================
  STEP #DENS#  Density Calculation
=================================================================
Transition density for SAC/SAC-CI (NV)
Threshold for S2 operators (CThreDensULS2):  0.00D+00
Threshold for R1,R2 operators (CThreDensULR1):  0.00D+00
Left and right vectors are used. (ILEFT=1)
```

```
-----------------------------------------------------------------------------------
Transition dipole moment of   triplet state from symmetry B1     1-th state
-----------------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
-----------------------------------------------------------------------------------
   A1         1      1.9287      0.1410      0.0000      0.0000      0.0009
   A1         2      8.1972     -0.0202      0.0000      0.0000      0.0001
   A2         1      2.4409      0.0000      1.5467      0.0000      0.1431
   A2         2     18.3010      0.0000      0.3353      0.0000      0.0504
   B1         1      0.0          Excitations are from this state.
   B1         2     15.9713      0.0000      0.0000      0.6484      0.1645
   B2         1      4.0226      0.0000      0.0000      0.0000      0.0000
   B2         2      6.3939      0.0000      0.0000      0.0000      0.0000
-----------------------------------------------------------------------------------
==================================================================
  STEP #CIMX#  CI matrix elements         ### IONIZED STATE ###
==================================================================
==================================================================
  STEP #DIAGCI#  Solution of SDCI
==================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Ionized   A1    CONVERGED
Solution for Ionized   B1    CONVERGED
Solution for Ionized   B2    CONVERGED
==================================================================
  STEP #ULINTIA#  Unlinked integral for Ionized State (SAC-CI)
==================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.000D+00 0.000D+00
Threshold for S2 operators (CThreULS2) 0.000D+00
==================================================================
  STEP #SCINV#  Iterative Diagonalization of SAC-CI-NV
==================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
-- Right vectors --
Solution for   1-th A1     CONVERGED
Solution for   2-th A1     CONVERGED
Solution for   3-th A1     CONVERGED
-- Left vectors --
Solution for   1-th A1     CONVERGED
Solution for   2-th A1     CONVERGED
Solution for   3-th A1     CONVERGED
-- Right vectors --
Solution for   1-th B1     CONVERGED
-- Left vectors --
Solution for   1-th B1     CONVERGED
-- Right vectors --
```

Transition dipole moments and oscillator strengths of the triplet excited states are summarized. The lowest state in triplet symmetry is used for the ground state.

Result of SAC-CI calculation for the ionized (cation doublet) state. Total energy, correlation energy (HF energy as the reference), excitation energy (SAC total energy as the reference), and the SAC-CI coefficients are shown. For example, the first ionized state in A_1 symmetry is the ionization from 4-th MO, and its ionization potential is 13.41 eV.

```
Solution for   1-th B2     CONVERGED
-- Left vectors --
Solution for   1-th B2     CONVERGED
***********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
***********************************************
***************************************************
CationDoublet A1      ****************************
###   1-st  ###           ---   2nd state in this spin multiplicity ---
    Total energy       in au =     -75.663487
    Correlation energy in au =       0.346351
    Excitation energy  in au =       0.492767    in eV =      13.408882
  *SINGLE EXCITATION
       4     0.97611         2     0.03353
  *DOUBLE EXCITATION
       4    9    4    -0.14069         3    7    4    -0.11896
       5    8    4    -0.10461         4    6    4    -0.07332
       3   12    4     0.06505         3   10    4    -0.05149
       2    6    4     0.04858         2   13    4    -0.03915
       4   11    4     0.03548         3   12    2     0.03257
       3    7    2    -0.03076
###   2-nd  ###           ---   4th state in this spin multiplicity ---
    Total energy       in au =     -74.886760
    Correlation energy in au =       1.123078
    Excitation energy  in au =       1.269495    in eV =      34.544708
  *SINGLE EXCITATION
       2    -0.43151
  *DOUBLE EXCITATION
       4    6    4    -1.09834         4   11    4     0.25845
       4    6    2     0.22051         3    6    3     0.20188
       4    9    4    -0.18832         4    7    3    -0.17913
       4   13    4     0.14803         2    6    4     0.13760
       4    9    2     0.10357         3   11    3    -0.09579
       4   11    2    -0.08085         3    7    4     0.07998
       4   12    3     0.06473         2    9    4     0.05627
       5    8    4     0.05258         5    8    2     0.04717
       3   12    4    -0.04627         2   11    4    -0.04224
       3    9    3     0.03956         4   10    3    -0.03830
       5    9    5     0.03010
###   3-rd  ###           ---   5th state in this spin multiplicity ---
    Total energy       in au =     -74.718158
    Correlation energy in au =       1.291680
    Excitation energy  in au =       1.438097    in eV =      39.132598
  *SINGLE EXCITATION
       2    -0.33426
  *DOUBLE EXCITATION
       4    7    3    -0.90462         3    7    4    -0.52887
       4    6    4     0.47163         4   12    3     0.32121
       3   12    4     0.19724         3    6    3    -0.17656
```

```
      4   10    3    -0.16704         4    8    5    -0.13389
      5    6    5     0.11509         4   13    4    -0.08264
      3   10    4    -0.08052         4    6    2     0.07283
      5    9    5     0.06815         2    6    2    -0.06544
      5    8    4    -0.05839         4   11    4    -0.05040
      5    8    2     0.04531         3    9    3    -0.04435
      4   11    2    -0.04116         3    7    2     0.03968
      2    7    3     0.03796
*******************************************************************************
CationDoublet B1      ******************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    Total energy       in au =     -75.728794
    Correlation energy in au =       0.281043
    Excitation energy  in au =       0.427460    in eV =      11.631777
  *SINGLE EXCITATION
      5    -0.97481
  *DOUBLE EXCITATION
      5    8    5     0.14766         3    7    5     0.11809
      4    9    5     0.10936         2    6    5    -0.07214
      3   12    5    -0.07116         4    6    5     0.05926
      3   10    5     0.05774         2   13    5     0.04333
      5    6    2    -0.03595         5    7    3     0.03215
      5   11    2     0.03174         2   11    5     0.03147
*******************************************************************************
CationDoublet B2      ******************************************************
###   1-st  ###           ---   3rd state in this spin multiplicity ---
    Total energy       in au =     -75.464478
    Correlation energy in au =       0.545360
    Excitation energy  in au =       0.691777    in eV =      18.824197
  *SINGLE EXCITATION
      3     0.98376
  *DOUBLE EXCITATION
      3    7    3    -0.09203         5    8    3    -0.09195
      4    9    3    -0.08694         3   10    3    -0.07479
      2    6    3     0.04817         4    7    2    -0.04008
      4   12    2     0.03967         2   13    3    -0.03625
      3   11    2     0.03481         5    7    5    -0.03143
==============================================================
  STEP #SATEI#  Monopole Intensity Calculation
==============================================================
Symmetry  State     I.P.        Intensity
-------------------------------------------
A1          1      13.409       0.95392
            2      34.545       0.18681
            3      39.133       0.11180
-------------------------------------------
B1          1      11.632       0.95026
-------------------------------------------
B2          1      18.824       0.96779
```

Monopole intensity for the ionizations. This is approximated intensity for the ionization spectrum.

```
-----------------------------------------
==============================================================
  STEP #DENS#  Density Calculation
==============================================================
Transition density for SAC/SAC-CI (NV)
Threshold for S2 operators (CThreDensULS2):  0.00D+00
Threshold for R1,R2 operators (CThreDensULR1):  0.00D+00
Left and right vectors are used. (ILEFT=1)
-----------------------------------------------------------------------------------
Transition dipole moment of   ionized state from symmetry B1     1-th state
-----------------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
-----------------------------------------------------------------------------------
   A1         1      1.7771     -0.1919      0.0000      0.0000      0.0016
   A1         2     22.9129      0.2647      0.0000      0.0000      0.0393
   A1         3     27.5008      0.1943      0.0000      0.0000      0.0254
   B1         1      0.0          Excitations are from this state.
   B2         1      7.1924      0.0000      0.0000      0.0000      0.0000
-----------------------------------------------------------------------------------
==============================================================
  STEP #CIMX#  CI matrix elements           ### ANION STATE ###
==============================================================
==============================================================
  STEP #DIAGCI#  Solution of SDCI
==============================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Anionized A1    CONVERGED
Solution for Anionized B1    CONVERGED
Solution for Anionized B2    CONVERGED
==============================================================
  STEP #ULINTIA#  Unlinked integral for Anionized State (SAC-CI)
==============================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.000D+00 0.000D+00
Threshold for S2 operators (CThreULS2) 0.000D+00
==============================================================
  STEP #SCINV#  Iterative Diagonalization of SAC-CI-NV
==============================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
-- Right vectors --
Solution for   1-th A1     CONVERGED
Solution for   2-th A1     CONVERGED
-- Left vectors --
Solution for   1-th A1     CONVERGED
Solution for   2-th A1     CONVERGED
-- Right vectors --
Solution for   1-th B1     CONVERGED
```

Transition dipole moments and oscillator strengths of the ionized (cation doublet) states are summarized. The lowest state in the ionized states is used for the ground state.

```
-- Left vectors --
Solution for   1-th B1     CONVERGED
-- Right vectors --
Solution for   1-th B2     CONVERGED
Solution for   2-th B2     CONVERGED
-- Left vectors --
Solution for   1-th B2     CONVERGED
Solution for   2-th B2     CONVERGED
***********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
***********************************************
*****************************************************************************
AnionDoublet  A1      ******************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    Total energy       in au =     -75.959222
    Correlation energy in au =       0.050616
    Excitation energy  in au =       0.197033    in eV =       5.361534
  *SINGLE EXCITATION
       6     0.98836
  *DOUBLE EXCITATION
       3    6    7    -0.07366         4    7    7    -0.06908
       5    8    6     0.06443         4    9    6     0.03909
       3   11    7     0.03185
###   2-nd  ###           ---   5th state in this spin multiplicity ---
    Total energy       in au =     -75.318506
    Correlation energy in au =       0.691332
    Excitation energy  in au =       0.837749    in eV =      22.796300
  *SINGLE EXCITATION
       9    -0.68494        11     0.06106
  *DOUBLE EXCITATION
       4    7    7    -0.82344         4    6    6    -0.29851
       3    7    6    -0.27881         3    6    7    -0.24816
       2    6    6     0.14414         4    6    9    -0.12989
       3    7    9    -0.10742         4    7   12     0.10080
       5    6    8    -0.09180         5    8    9    -0.07480
       4   12    7     0.06403         5    8    6    -0.05427
       4    9    9    -0.05060         3    6   12     0.05054
       2    6    9     0.04846         3    7   11     0.04814
       2    7    7     0.04621         3   10    6    -0.04362
       4    6   11     0.04118         4   10    7    -0.03913
       4    7   10    -0.03713         2    6   11    -0.03562
       3    6   10    -0.03502         4   12   12     0.03226
*****************************************************************************
AnionDoublet  B1      ******************************************************
###   1-st  ###           ---   4th state in this spin multiplicity ---
    Total energy       in au =     -75.321567
    Correlation energy in au =       0.688271
    Excitation energy  in au =       0.834688    in eV =      22.713010
  *SINGLE EXCITATION
```

Result of SAC-CI method for the electron-attached (anion doublet) state. Total energy, correlation energy (HF energy as the reference), excitation energy (SAC total energy as the reference), and the SAC-CI coefficients are shown. For example, the first electron-attached state in A_1 symmetry is the electron-attachment to 6-th MO, and its vertical electron affinity is 5.36 eV.

```
      8    -0.97049
  *DOUBLE EXCITATION
      5    8    8    -0.13987         5    7    7     0.12610
      3    7    8    -0.12131         4    6    8    -0.09690
      4    9    8    -0.08829         5    6    6     0.06482
      2    6    8     0.06424         5   11    6     0.03666
*****************************************************************************
AnionDoublet  B2      ***************************************************
###   1-st  ###           ---   2nd state in this spin multiplicity ---
    Total energy       in au =     -75.870687
    Correlation energy in au =       0.139151
    Excitation energy  in au =       0.285568    in eV =       7.770690
  *SINGLE EXCITATION
      7     0.98345
  *DOUBLE EXCITATION
      3    6    6    -0.11022         4    7    6    -0.08990
      5    8    7     0.07384         4    9    7     0.05230
      3   11    6     0.03833         5    8   12    -0.03694
      3    7   12    -0.03637         4    9   12    -0.03346
      3   10    7     0.03205         3    7    7     0.03110
###   2-nd  ###           ---   3rd state in this spin multiplicity ---
    Total energy       in au =     -75.409369
    Correlation energy in au =       0.600469
    Excitation energy  in au =       0.746886    in eV =      20.323791
  *SINGLE EXCITATION
     10    -0.10896         7     0.10676
     12     0.04137
  *DOUBLE EXCITATION
      3    6    6     1.14870         4    7    6     0.44812
      3    7    7    -0.32928         2    6    7    -0.09100
      3    6   11    -0.07863         4    6    7    -0.06396
      2    7    6    -0.06340         3    6   13    -0.04270
      2    6   12     0.04137         4    6   10    -0.04012
      3    7   10    -0.03732         4   10    6     0.03561
      5    8    7     0.03247         3   13    6    -0.03212
==============================================================
  STEP #DENS#  Density Calculation
==============================================================
Transition density for SAC/SAC-CI (NV)
Threshold for S2 operators (CThreDensULS2):  0.00D+00
Threshold for R1,R2 operators (CThreDensULR1):  0.00D+00
Left and right vectors are used. (ILEFT=1)
-----------------------------------------------------------------------------
Transition dipole moment of anionized state from symmetry A1     1-th state
-----------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
-----------------------------------------------------------------------------
   A1         1      0.0          Excitations are from this state.
```

Transition dipole moments and oscillator strengths of the electron-attached (anion doublet) states are summarized. The lowest state in the electron-attached states is used for the ground state.

```
   A1          2      17.4348      0.0000      0.0000     -0.7475      0.2387
   B1          1      17.3515     -0.6790      0.0000      0.0000      0.1960
   B2          1       2.4092      0.0000      1.4252      0.0000      0.1199
   B2          2      14.9623      0.0000      1.0397      0.0000      0.3963
-------------------------------------------------------------------------------
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.

*********************************************************************

           Population analysis using the SCF density.

*********************************************************************

Orbital symmetries:
      Occupied  (A1) (A1) (B2) (A1) (B1)
      Virtual   (A1) (B2) (B1) (A1) (B2) (A1) (B2) (A1) (A1)
The electronic state is 1-A1.
Alpha  occ. eigenvalues --  -20.55815  -1.34595  -0.71723  -0.55296  -0.50247
Alpha virt. eigenvalues --    0.21403   0.30615   0.86755   0.89179   0.94327
Alpha virt. eigenvalues --    1.16931   1.22707   1.65220  43.32907
         Condensed to atoms (all electrons):
             1          2          3
    1  O    8.236019   0.279375   0.279375
    2  H    0.279375   0.353639  -0.030398
    3  H    0.279375  -0.030398   0.353639
Mulliken atomic charges:
             1
    1  O   -0.794768
    2  H    0.397384
    3  H    0.397384
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  O    0.000000
    2  H    0.000000
    3  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    19.5527
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     0.0000    Y=     0.0000    Z=    -2.5778  Tot=     2.5778
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -7.4356   YY=    -3.8859   ZZ=    -6.4290
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -1.5188   YY=     2.0310   ZZ=    -0.5122
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
```

```
 XXX=     0.0000  YYY=     0.0000  ZZZ=    -1.5928  XYY=     0.0000
 XXY=     0.0000  XXZ=    -0.4528  XZZ=     0.0000  YZZ=     0.0000
 YYZ=    -1.4398  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=    -5.8335 YYYY=    -5.5689 ZZZZ=    -6.6383 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=    -2.2132 XXZZ=    -2.1180 YYZZ=    -1.7716
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 9.009354229663D+00 E-N=-1.986615255635D+02  KE= 7.597667007820D+01
Symmetry A1   KE= 6.795191278244D+01
Symmetry A2   KE= 0.000000000000D+00
Symmetry B1   KE= 4.545680221158D+00
Symmetry B2   KE= 3.479077074604D+00

Test job not archived.
1¥1¥GINC-MIRAI86¥SP¥RSACCI¥D95¥H2O1¥MASAHIRO¥31-Jul-2004¥0¥¥# SAC-CI(S
INGLET=(NSTATE=(2,2,2,2),NONVARIATIONAL), TRIPLET=(NSTATE=(2,2,2,2),NO
NVARIATIONAL), CATIONDOUBLET=(NSTATE=(3,0,1,1),NONVARIATIONAL), ANIOND
OUBLET=(NSTATE=(2,0,1,2),NONVARIATIONAL), FULLACTIVE, SD-R, NOLINKEDSE
LECTION, NOUNLINKEDSELECTION) /D95 UNIT=BOHR TEST¥¥Gaussian Test Job 6
31: SAC-CI SD-R NV calculations for singlet, triplet, ionized, and ele
ctron-attached states of H2O with Huzinaga-Dunning D95 basis. All the
SCF MOs are included in the active space (FullActive) and SAC-CI calcu
lations are performed without selections (NoLinkedSelection, NoUnLinke
dSelection). The results are compared with the full-CI results calcula
ted separately. See PartI-L of the SAC-CI Guide. Reference: N. C. Hand
y, Chem. Phys. Lett. 74, 280 (1980); H. Nakatsuji, K. Hirao, Y. Mizuka
mi, Chem. Phys. Lett. 179, 555 (1991).¥¥0,1¥O,0,0.,0.,0.¥H,0,0.8018426
442,0.,-0.5555820926¥H,0,-0.8018426442,0.,-0.5555820926¥¥Version=AI64T
-G03RevC.02¥State=1-A1¥HF=-76.0098376¥RMSD=5.275e-10¥PG=C02V [C2(O1),S
GV(H2)]¥¥@


COLLEGE PROFESSOR: SOMEONE WHO TALKS IN OTHER PEOPLE'S SLEEP.
Job cpu time:  0 days  0 hours  0 minutes 25.0 seconds.
File lengths (MBytes):  RWF=    484 Int=      0 D2E=      0 Chk=     10 Scr=     28
Normal termination of Gaussian 03 at Sat Jul 31 11:45:59 2004.
```

Output 635

```
Entering Gaussian System, Link 0=/work/g03.C02/g03/g03
Initial command:
/work/g03.C02/g03/l1.exe /work/g03.C02/inputs/Gau-113434.inp -scrdir=/work/g03.C02/inputs/
Entering Link 1 = /work/g03.C02/g03/l1.exe PID=    113433.

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```

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Gaussian 03, Revision C.02,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,

```
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,
A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

******************************************
Gaussian 03:  AI64T-G03RevC.02 12-Jun-2004
               31-Jul-2004
******************************************
%mem=12mw
---------------------------------------------------------------------------
# SAC-CI(LevelOne, Singlet=(NState=(2,3,3,1,2,2,2,5)), Triplet=(NState
=(2,3,3,1,2,2,2,5)), CationDoublet=(NState=(2,0,0,1,0,1,1,1))) /Gen Ma
ssage Symm=On test
---------------------------------------------------------------------------
1/38=1/1;
2/15=-1,17=6,18=5,40=1/2;
3/5=7,10=10,11=9,16=1,25=1,30=1,36=2/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=5,9=30000,10=1,40=1,42=2/1,4;
9//23;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;
---------------------------------------------------------------------------
Gaussian Test Job 635 (Part 1): Comparison of LevelOne, LevelTwo, and
LevelThree calculations for ethylene. First is LevelOne calculation. S
AC-CI SD-R calculations for singlet, triplet, and ionized states of et
hylene using Huzinaga-Dunning basis with polarization functions [4s2p1
d/2s1p] plus Rydberg functions [2s2p2d] on center of molecule. Inner-s
hells are excluded from the active space and full-valence active MOs a
re used (FC; default). Dummy atom is used with symmetry (Massage,Symm=
On). The results are summarized in Part I-L of the SAC-CI Guide.
---------------------------------------------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
```

List of keywords given in the Gaussian input

Nuclear coordinates for C_2H_4 given in the Gaussian input

```
H1
C2                  1    r1
C3                  2    r2       1    a1
H4                  3    r1       2    a1       1     0.       0
H5                  3    r1       2    a1       1     180.     0
H6                  2    r1       3    a1       4     180.     0
N7                  2    r22      1    a1       4     0.       0
     Variables:
 r1                   1.0868
 r2                   1.3391
 a1                 121.28
 r22                  0.66955
```

Dummy atom (nitrogen) at the center of C=C bond. This is to define the bond-centered diffuse functions. Later step clear its nuclear charge.

```
                        Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          1           0        0.000000    0.000000    0.000000
   2          6           0        0.000000    0.000000    1.086800
   3          6           0        1.144449    0.000000    1.782089
   4          1           0        2.108977    0.000000    1.281270
   5          1           0        1.144449    0.000000    2.868889
   6          1           0       -0.964528    0.000000    1.587619
   7          7           0        0.572224    0.000000    1.434444
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  H    0.000000
    2  C    1.086800   0.000000
    3  C    2.117924   1.339100   0.000000
    4  H    2.467678   2.117924   1.086800   0.000000
    5  H    3.088735   2.117924   1.086800   1.857646   0.000000
    6  H    1.857646   1.086800   2.117924   3.088735   2.467678
    7  N    1.544368   0.669550   0.669550   1.544368   1.544368
                  6          7
    6  H    0.000000
    7  N    1.544368   0.000000
Stoichiometry    C2H4N
Framework group  D2H[O(N),C2"(C.C),SG(H4)]
Deg. of freedom     3
Full point group                 D2H     NOp   8
Largest Abelian subgroup         D2H     NOp   8
Largest concise Abelian subgroup D2      NOp   4
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
```

Nuclear coordinates used in the actual calculation

```
   1          1             0        0.000000     0.928823     1.233839
   2          6             0        0.000000     0.000000     0.669550
   3          6             0        0.000000     0.000000    -0.669550
   4          1             0        0.000000     0.928823    -1.233839
   5          1             0        0.000000    -0.928823    -1.233839
   6          1             0        0.000000    -0.928823     1.233839
   7          7             0        0.000000     0.000000     0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     145.3135944      29.9107742      24.8050094
General basis read from cards:  (5D, 7F)
The nuclear charge for atom    7 has been changed to Z=  0   0.000000
There are    18 symmetry adapted basis functions of AG  symmetry.
There are     4 symmetry adapted basis functions of B1G symmetry.
There are     6 symmetry adapted basis functions of B2G symmetry.
There are     9 symmetry adapted basis functions of B3G symmetry.
There are     2 symmetry adapted basis functions of AU  symmetry.
There are    14 symmetry adapted basis functions of B1U symmetry.
There are     9 symmetry adapted basis functions of B2U symmetry.
There are     6 symmetry adapted basis functions of B3U symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   68 basis functions,   108 primitive gaussians,    72 cartesian basis functions
    8 alpha electrons        8 beta electrons
      nuclear repulsion energy        33.2499942363 Hartrees.
NAtoms=    7 NActive=    7 NUniq=    3 SFac= 5.66D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    68 RedAO= T  NBF=    18     4     6     9     2    14     9     6
NBsUse=    68 1.00D-06 NBFU=    18     4     6     9     2    14     9     6
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.13D-02 ExpMax= 4.23D+03 ExpMxC= 6.35D+02 IAcc=3 IRadAn=         5 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=         5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Warning:  off-atom basis functions, so minimal bfn integration tests in XC quadrature.
Initial guess orbital symmetries:
      Occupied  (AG) (B1U) (AG) (B1U) (B2U) (AG) (B3G) (B3U)
      Virtual   (B2G) (AG) (B2U) (B1U) (B3U) (AG) (B3G) (AG) (B2G)
                (B1G) (AG) (B2U) (B1U) (B3G) (AG) (B1G) (AG) (B3U)
                (B2G) (B2U) (B1U) (AG) (B1U) (AG) (B3G) (B2U)
                (B2G) (B3U) (B1U) (B3G) (AG) (B1U) (B2U) (AG)
                (B1U) (B1G) (B3U) (B3G) (AU) (AG) (AG) (B3G) (B2U)
                (B1U) (B2G) (B2U) (B3U) (B1U) (B1G) (B2G) (AU)
                (AG) (B3G) (B1U) (AG) (B2U) (B1U) (B3G) (AG) (B1U)
The electronic state of the initial guess is 1-AG.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=     4505542.
```

Clear charge of the dummy nucleus “N”

```
SCF Done:  E(RHF) =  -78.0508720221     A.U. after    9 cycles
            Convg  =    0.3635D-08             -V/T =  2.0026
            S**2   =   0.0000
ExpMin= 1.13D-02 ExpMax= 4.23D+03 ExpMxC= 6.35D+02 IAcc=3 IRadAn=        5 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=        5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Warning:  off-atom basis functions, so minimal bfn integration tests in XC quadrature.
Range of M.O.s used for correlation:     3    68
NBasis=    68 NAE=     8 NBE=     8 NFC=     2 NFV=     0
NROrb=     66 NOA=     6 NOB=     6 NVA=    60 NVB=    60
-----------------------------------------------------------------------
#######################################################################
-----------------------------------------------------------------------
```

Hartree-Fock SCF energy.

AO to MO transformation of two-electron repulsion integrals

```
              SAC/SAC-CI Program Combined with GAUSSIAN
                              for Calculating
        Ground, Excited, Ionized, and Electron-Attached States
                                 and
             Singlet, Doublet, Triplet, Quartet, Quintet,
                    Sextet, and Septet Spin States
                                 and
                  Their Analytical Energy Gradients
                         coded originally by
                          Hiroshi Nakatsuji
                           and extended by
 H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa,
      M. Ishida, T. Nakajima, Y. Honda, O. Kitao, and H. Nakai
                                 at
                  Department of Hydrocarbon Chemistry,
                Division of Molecular Engineering, and
      Department of Synthetic Chemistry & Biological Chemistry,
                   Graduate School of Engineering,
                          Kyoto University,
                        Kyoto 606-8501, Japan
-----------------------------------------------------------------------
#######################################################################
-----------------------------------------------------------------------
No. of INTEGRALS =    324236 NBLK =       202 KOUNT =      1036
###########################################################################
    Singles-Doubles (SD) SAC/SAC-CI  (SAC-CI SD-R)
###########################################################################
==============================================================
  STEP #PRES#  Generation of Linked Operators and Selection
==============================================================
== States to be calculated ==
           AG   B1G  B2G  B3G  AU   B1U  B2U  B3U
SINGLET    Yes  Yes  Yes  Yes  Yes  Yes  Yes  Yes
TRIPLET    Yes  Yes  Yes  Yes  Yes  Yes  Yes  Yes
IONIZED    Yes  Yes  Yes  Yes  Yes  Yes  Yes  Yes
ANIONIZED  No   No   No   No   No   No   No   No
```

Beginning of the SAC-CI part of the program

```
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  3,  3,  3,  1,  2,  2,  2,  5)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelOne #
  EThreS2 (Lambda_G)=  0.100D-04(au)   EThreR2 (Lambda_E)=  0.100D-05(au)
TRIPLET STATE
 Number of States  Triplet      =(  2,  3,  3,  1,  2,  2,  2,  5)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelOne #
  EThreR2 (Lambda_E)=  0.100D-05(au)
IONIZED STATE
 Number of States  CationDoublet=(  2,  0,  0,  1,  0,  1,  1,  1)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelOne #
  EThreR2 (Lambda_E)=  0.100D-05(au)
****************************
        SINGLET STATE
****************************
------------------------------------------------------------
LINKED OPERATORS FOR SAC:    SYMMETRY = AG  GROUND STATE
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            63        9024         9087
    AFTER             63        2763         2827
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AG  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.296334
       8 ->  17     0.94023        8 ->  25     0.32851
    ##   2-nd state ##       energy (au) =       0.380223
       8 ->  25     0.92052        8 ->  17    -0.33907
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            63        9024         9087
    AFTER             63        1447         1511
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.281843
       8 ->  11     0.86335        8 ->  23     0.48630
       8 ->  29     0.10227
    ##   2-nd state ##       energy (au) =       0.341571
       7 ->  18     0.72120        7 ->  27    -0.64239
       7 ->  14     0.14162        8 ->  23     0.11167
       7 ->  36    -0.11143        8 ->  11    -0.11010
    ##   3-th state ##       energy (au) =       0.356963
       8 ->  23     0.82116        8 ->  11    -0.49204
       8 ->  29     0.19651        8 ->  34    -0.12686
       7 ->  18    -0.12591        7 ->  27     0.10502
  SELECTION        SINGLE      DOUBLE       TOTAL
```

Number of the linked operators for single- and double- excitations before and after the perturbation selection

Main configurations of the reference SECI calculation used for the perturbation selection step. For example, the first excited state in singlet A_g symmetry is the transition from 8-th MO to 17-th MO, and its CI coefficient is about 0.94.

```
    BEFORE            29        7364         7393
    AFTER             29        2845         2874
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.287373
       8 ->  10     0.91243        8 ->  24     0.39911
    ##   2-nd state ##       energy (au) =       0.369257
       8 ->  24     0.81584        8 ->  10    -0.38382
       6 ->  27    -0.27427        6 ->  18     0.26566
       8 ->  31    -0.17400
    ##   3-th state ##       energy (au) =       0.376304
       6 ->  27     0.63715        6 ->  18    -0.62072
       8 ->  24     0.37166        6 ->  36     0.15588
       8 ->  10    -0.14036        6 ->  14    -0.10387
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            35        7484         7519
    AFTER             35        2803         2838
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.386987
       7 ->   9     0.87379        7 ->  26     0.37236
       7 ->  19    -0.16572        7 ->  16     0.14314
       5 ->  24     0.11788
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            53        8708         8761
    AFTER             53        1943         1996
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AU  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.320962
       8 ->  12     0.90268        8 ->  22     0.42641
    ##   2-nd state ##       energy (au) =       0.368854
       8 ->  22     0.89326        8 ->  12    -0.43030
       8 ->  33     0.12187
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            27        7356         7383
    AFTER             27        1141         1168
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.284181
       8 ->  18     0.82474        8 ->  27    -0.40146
       8 ->  14     0.33925
    ##   2-nd state ##       energy (au) =       0.331060
       8 ->  14     0.91523        8 ->  27     0.34202
       8 ->  18    -0.18352
  SELECTION        SINGLE      DOUBLE       TOTAL
```

```
    BEFORE            61        8836         8897
    AFTER             61        1867         1928
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.320792
       8 ->  15     0.88807        8 ->  20     0.45915
    ##   2-nd state ##       energy (au) =       0.364234
       8 ->  20     0.88703        8 ->  15    -0.45967
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            55        8716         8771
    AFTER             55         663          718
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.260350
       8 ->   9     0.89702        8 ->  26     0.35048
       8 ->  16     0.17828        8 ->  19    -0.16415
    ##   2-nd state ##       energy (au) =       0.315645
       8 ->  13     0.72791        8 ->  19     0.57881
       8 ->  16     0.34382        8 ->  28     0.11322
    ##   3-th state ##       energy (au) =       0.319844
       8 ->  16     0.77242        8 ->  21    -0.48071
       8 ->  13    -0.38277        8 ->   9    -0.14211
    ##   4-th state ##       energy (au) =       0.348811
       8 ->  19     0.65807        8 ->  13    -0.49993
       8 ->   9     0.34671        8 ->  26    -0.34490
       8 ->  28     0.20148        8 ->  16    -0.17875
    ##   5-th state ##       energy (au) =       0.361679
       8 ->  21     0.82835        8 ->  16     0.46809
       8 ->  26    -0.20355        8 ->  19    -0.13967
       8 ->  13    -0.13875
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            37        7492         7529
    AFTER             37        2137         2174
*****************************
        TRIPLET STATE
*****************************
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AG  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.284276
       8 ->  17     0.86842        8 ->  25     0.48460
    ##   2-nd state ##       energy (au) =       0.363288
       8 ->  25     0.85196        8 ->  17    -0.49556
       8 ->  35    -0.15070
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            63       12189        12252
    AFTER             63        1214         1277
```

Main configurations of the reference SECI calculation used for the perturbation selection step. For example, the first excited state in triplet A_g symmetry is the transition from 8-th MO to 17-th MO, and its CI coefficient is about 0.87.

```
-----------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.278966
       8 ->  11     0.83989        8 ->  23     0.51633
       8 ->  29     0.12821
    ##   2-nd state ##       energy (au) =       0.316463
       7 ->  18     0.70581        7 ->  27    -0.67742
       7 ->  14     0.12567        7 ->  36    -0.12532
    ##   3-th state ##       energy (au) =       0.352620
       8 ->  23     0.79138        8 ->  11    -0.53814
       8 ->  29     0.24969        8 ->  34    -0.13223
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            29       10500        10529
    AFTER             29        3521         3550
-----------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.283348
       8 ->  10     0.88446        8 ->  24     0.44379
       8 ->  31    -0.13053
    ##   2-nd state ##       energy (au) =       0.347308
       6 ->  27     0.69974        6 ->  18    -0.64978
       6 ->  36     0.18078        8 ->  10     0.10859
       8 ->  24    -0.10797        6 ->  14    -0.10124
    ##   3-th state ##       energy (au) =       0.364354
       8 ->  24     0.84635        8 ->  10    -0.45313
       8 ->  31    -0.21638        6 ->  27     0.11741
       6 ->  18    -0.10643
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            35       10602        10637
    AFTER             35        3447         3482
-----------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.370044
       7 ->   9     0.77647        7 ->  26     0.44073
       7 ->  19    -0.21913        7 ->  28    -0.17447
       5 ->  24     0.17377        5 ->  10     0.11183
       7 ->  16     0.11173
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            53       12222        12275
    AFTER             53        2749         2802
-----------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AU  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.320525
       8 ->  12     0.89588        8 ->  22     0.43915
    ##   2-nd state ##       energy (au) =       0.367583
```

```
      8 ->  22     0.88376        8 ->  12    -0.44423
      8 ->  33     0.13093
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            27       10506        10533
    AFTER             27        1261         1288
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.129560
      8 ->  27     0.71782        8 ->  18    -0.66032
      8 ->  36     0.17938        8 ->  14    -0.10220
    ##   2-nd state ##       energy (au) =       0.324207
      8 ->  14     0.93866        8 ->  27     0.28541
      8 ->  18     0.18242
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            61       12318        12379
    AFTER             61        1812         1873
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.319743
      8 ->  15     0.86916        8 ->  20     0.49394
    ##   2-nd state ##       energy (au) =       0.361471
      8 ->  20     0.86729        8 ->  15    -0.49439
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            55       12240        12295
    AFTER             55         763          818
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.252381
      8 ->   9     0.85547        8 ->  26     0.42815
      8 ->  16     0.19023        8 ->  19    -0.16184
    ##   2-nd state ##       energy (au) =       0.313559
      8 ->  16     0.62658        8 ->  19     0.54898
      8 ->  13     0.40646        8 ->  21    -0.32387
      8 ->  28     0.15678
    ##   3-th state ##       energy (au) =       0.315979
      8 ->  13     0.68320        8 ->  21     0.49464
      8 ->  16    -0.38839        8 ->  19     0.26803
      8 ->   9     0.20236        8 ->  26    -0.11168
      8 ->  32     0.10498
    ##   4-th state ##       energy (au) =       0.345015
      8 ->  13     0.53277        8 ->  19    -0.50357
      8 ->  26     0.47087        8 ->   9    -0.39931
      8 ->  21    -0.20178        8 ->  28    -0.17378
    ##   5-th state ##       energy (au) =       0.350851
      8 ->  16     0.64554        8 ->  21     0.60356
      8 ->  19    -0.35868        8 ->  26    -0.20475
```

```
      8 ->  28    -0.16720        8 ->  32     0.11453
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            37       10593        10630
    AFTER             37        2553         2590
****************************
       IONIZED STATE
****************************
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AG  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.585304
       6     1.00000
    ##   2-nd state ##       energy (au) =       1.033118
       3     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             2         332          334
    AFTER              2         312          314
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.508192
       7     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1         312          313
    AFTER              1         256          257
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.792389
       4     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1         328          329
    AFTER              1         272          273
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.643034
       5     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1         316          317
    AFTER              1         264          265
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.374824
       8     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1         228          229
    AFTER              1         188          189
```

Main configurations of the reference SECI calculation used for the perturbation selection step. The first ionized (cation doublet) state in A_g symmetry is the ionization from 6-th MO, and its CI coefficient is about 1.00.

```
=================================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
=================================================================
=================================================================
  STEP #DIAGCI#  Solution of SDCI
=================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   AG    CONVERGED
Solution for Singlet   AG    CONVERGED
Solution for Singlet   B1G   CONVERGED
Solution for Singlet   B2G   CONVERGED
Solution for Singlet   B3G   CONVERGED
Solution for Singlet   AU    CONVERGED
Solution for Singlet   B1U   CONVERGED
Solution for Singlet   B2U   CONVERGED
Solution for Singlet   B3U   CONVERGED
=================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
=================================================================
Threshold for S2 operator (CThreULS2G) 0.500D-02
=================================================================
  STEP #SAC#  Solution of SAC equation
=================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-05
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Solution for SAC equation converged
*********************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*********************************************
HF ENERGY     =     -78.050872 (AU)
SAC-NV  ENERGY=      -0.261923 (AU)
TOTAL ENERGY  =     -78.312795 (AU)
SAC-NV  coefficients (|C|>=0.03)
*SINGLE EXCITATION
*DOUBLE EXCITATION
       8   27    8   18      0.11536         8   27    8   27     -0.08277
       8   36    8   27     -0.07595         8   36    8   18      0.04956
       8   27    6   38     -0.04788         8   18    8   18     -0.04106
       8   36    6   38     -0.03938         8   18    6   38      0.03039
Hartree-Fock configuration   1.00000
=====================================================================
  STEP #ULINTS#  Unlinked integral for Singlet Excited State (SAC-CI)
=====================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
```

Result of SAC calculation. Hartree-Fock (HF) energy, SAC-NV energy (correlation energy obtained with the SAC method), and the SAC-NV coefficients are shown. HF configuration always has 1.00 in the SAC wave function.

```
=================================================================
  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
=================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   AG    CONVERGED
Solution for Singlet   B1G   CONVERGED
Solution for Singlet   B2G   CONVERGED
Solution for Singlet   B3G   CONVERGED
Solution for Singlet   AU    CONVERGED
Solution for Singlet   B1U   CONVERGED
Solution for Singlet   B2U   CONVERGED
Solution for Singlet   B3U   CONVERGED
***********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
***********************************************
*****************************************************************************
Singlet       AG      ******************************************************
###   1-st  ###           ---   5th state in this spin multiplicity ---
    Total energy       in au =     -78.013090
    Correlation energy in au =       0.037782
    Excitation energy  in au =       0.299705    in eV =       8.155389
  *SINGLE EXCITATION
       8   17     0.91561         8   25     0.32586
  *DOUBLE EXCITATION
       8   25    8   17    -0.10502         8   35    8   17     0.08672
       8   17    7   33    -0.07065         8   17    5   29    -0.06464
       8   17    6   32    -0.06216         8   17    4   31     0.06015
       8   17    5   23    -0.05604         8   17    5   34     0.05211
       8   17    7   37     0.04839         8   36    8   27     0.04284
       8   27    8   27     0.03830         8   17    4   24    -0.03481
       8   17    7   22    -0.03409         8   25    8   25    -0.03243
       8   17    8   17    -0.03075
###   2-nd  ###           ---  20th state in this spin multiplicity ---
    Total energy       in au =     -77.927800
    Correlation energy in au =       0.123072
    Excitation energy  in au =       0.384995    in eV =      10.476251
  *SINGLE EXCITATION
       8   25     0.90090         8   17    -0.33504
       8   35    -0.08938         7   22    -0.06853
       6    9    -0.05244         7   33    -0.03051
  *DOUBLE EXCITATION
       8   25    8   25    -0.09049         8   35    8   25     0.08879
       8   36    8   27     0.07328         8   25    7   33    -0.06186
       8   27    8   27     0.05536         8   25    5   29    -0.05451
       8   25    6   32    -0.05382         8   25    4   31     0.05270
       8   27    8   18    -0.05109         8   36    8   18    -0.04559
       8   25    5   23    -0.03915         8   25    5   34     0.03914
       8   25    7   37     0.03455         8   35    8   17    -0.03085
```

Result of SAC-CI calculation. Total energy, correlation energy (HF energy as the reference), excitation energy (SAC total energy as the reference), and the SAC-CI coefficients are shown. For example, the first excited state in singlet A_g symmetry is the excitation from 8-th MO to 17-th MO, and its excitation energy is 8.16 eV.

```
      8   25    4   24    -0.03047
*****************************************************************************
Singlet       B1G     ***********************************************************
###   1-st  ###           ---   2nd state in this spin multiplicity ---
    Total energy       in au =     -78.026291
    Correlation energy in au =       0.024581
    Excitation energy  in au =       0.286504    in eV =       7.796160
  *SINGLE EXCITATION
      8   11     0.85063         8   23     0.46193
      8   29     0.08682         8   34    -0.06986
      7   18     0.04173         7   27    -0.03915
  *DOUBLE EXCITATION
      8   25    8   11    -0.08323         8   35    8   11     0.07751
      8   11    7   33    -0.06547         8   11    5   29    -0.06053
      8   11    6   32    -0.05774         8   11    4   31     0.05688
      8   11    5   23    -0.05278         8   11    5   34     0.04146
      8   25    8   23    -0.04058         8   11    7   37     0.03886
      8   35    8   23     0.03592         8   11    4   24    -0.03244
      8   11    7   22    -0.03222         8   33    8   27     0.03091
      8   23    7   33    -0.03007
###   2-nd  ###           ---   8th state in this spin multiplicity ---
    Total energy       in au =     -77.988618
    Correlation energy in au =       0.062254
    Excitation energy  in au =       0.324177    in eV =       8.821309
  *SINGLE EXCITATION
      7   18     0.71525         7   27    -0.61652
      7   14     0.14197         7   36    -0.11212
      8   11    -0.08988         8   29     0.05661
  *DOUBLE EXCITATION
      8   27    5   18    -0.11806         8   27    5   27     0.10991
      8   18    5   18     0.09187         8   18    5   27    -0.09109
      8   36    5   18    -0.03996         7   30    4   27     0.03642
      7   30    4   18    -0.03618         8   35    7   36     0.03446
      7   29    5   18     0.03305         7   43    4   27    -0.03264
      6   38    5   18    -0.03216         7   43    4   18     0.03212
      7   29    5   27    -0.03204         8   36    5   27     0.03047
###   3-rd  ###           ---  14th state in this spin multiplicity ---
    Total energy       in au =     -77.948977
    Correlation energy in au =       0.101895
    Excitation energy  in au =       0.363818    in eV =       9.899980
  *SINGLE EXCITATION
      8   23    -0.82505         8   11     0.46948
      8   29    -0.17782         8   34     0.12280
      7   18     0.06486         7   27    -0.04410
  *DOUBLE EXCITATION
      8   25    8   23     0.07450         8   35    8   23    -0.06808
      8   23    7   33     0.05552         8   23    5   29     0.05320
      8   23    4   31    -0.05104         8   25    8   11    -0.05005
      8   35    8   11     0.04746         8   33    8   27    -0.04387
```

```
      8   23    5   23     0.04145         8   23    6   32     0.04075
      8   11    7   33    -0.04016         8   23    5   34    -0.03665
      8   11    5   29    -0.03652         8   11    6   32    -0.03621
      8   11    4   31     0.03374         8   23    7   37    -0.03339
      8   11    5   23    -0.03164
*****************************************************************************
Singlet       B2G     ******************************************************
###   1-st  ###           ---   3rd state in this spin multiplicity ---
    Total energy       in au =     -78.025391
    Correlation energy in au =       0.025481
    Excitation energy  in au =       0.287404    in eV =       7.820661
  *SINGLE EXCITATION
      8   10     0.87398         8   24     0.41688
      8   31    -0.09181
  *DOUBLE EXCITATION
      8   25    8   10    -0.08511         8   35    8   10     0.07931
      8   10    7   33    -0.06744         8   10    5   29    -0.06735
      8   10    6   32    -0.06290         8   10    4   31     0.06159
      8   10    5   23    -0.05309         8   10    7   37     0.04940
      8   10    5   34     0.04107         8   27    8    9     0.04097
      8   26    8   18    -0.04054         8   27    8   26     0.03987
      8   25    8   24    -0.03709         8   10    4   24    -0.03529
      8   10    7   22    -0.03368         8   24    5   29    -0.03311
      8   35    8   24     0.03305         8   18    8    9    -0.03004
###   2-nd  ###           ---  16th state in this spin multiplicity ---
    Total energy       in au =     -77.943804
    Correlation energy in au =       0.107068
    Excitation energy  in au =       0.368990    in eV =      10.040738
  *SINGLE EXCITATION
      8   24     0.71216         8   10    -0.38076
      6   18     0.36536         6   27    -0.34020
      8   31    -0.17557         6   36    -0.07517
      6   14     0.06424         8   30    -0.05219
  *DOUBLE EXCITATION
      8   25    8   24    -0.06534         8   27    8   26     0.06292
      8   35    8   24     0.05997         8   26    8   18    -0.05412
      8   24    5   29    -0.05388         8   27    4   27     0.05127
      8   24    7   33    -0.04987         8   24    6   32    -0.04971
      8   27    4   18    -0.04956         8   24    4   31     0.04910
      8   25    8   10     0.04074         8   35    8   10    -0.03864
      8   18    4   27    -0.03349         8   24    5   23    -0.03254
      8   10    7   33     0.03239         8   24    7   37     0.03218
      8   18    4   18     0.03194         8   24    4   24    -0.03072
      8   32    8   27     0.03026         8   24    5   34     0.03017
      8   27    8    9     0.03002
###   3-rd  ###           ---  19th state in this spin multiplicity ---
    Total energy       in au =     -77.936797
    Correlation energy in au =       0.114075
    Excitation energy  in au =       0.375998    in eV =      10.231419
```

```
  *SINGLE EXCITATION
       6   18    -0.59416         6   27     0.55000
       8   24     0.46936         8   10    -0.20356
       6   36     0.12171         6   14    -0.11046
       3   27    -0.05152         8   31    -0.04931
       3   18     0.03227
  *DOUBLE EXCITATION
       8   27    4   18     0.06185         8   27    4   27    -0.05313
       8   18    4   18    -0.05249         8   18    4   27     0.04907
       8   25    8   24    -0.04475         8   35    8   24     0.04115
       8   24    5   29    -0.03584         8   27    8   26     0.03445
       8   24    7   33    -0.03364         8   24    4   31     0.03191
       6   38    4   18     0.03142         6   38    4   27    -0.03081
       8   26    8   18    -0.03052
*****************************************************************************
Singlet       B3G     ***********************************************************
###   1-st  ###           ---  13th state in this spin multiplicity ---
    Total energy       in au =     -77.954702
    Correlation energy in au =       0.096170
    Excitation energy  in au =       0.358093    in eV =       9.744209
  *SINGLE EXCITATION
       7    9    -0.87502         7   26    -0.34007
       7   19     0.16080         7   16    -0.13025
       7   28     0.06934         7   13    -0.06322
  *DOUBLE EXCITATION
       8   27    5    9     0.12154         8   18    5    9    -0.08326
       8   35    7    9    -0.06785         8   25    7    9     0.06723
       8   36    5    9     0.06027         7   33    7    9     0.05060
       8   27    5   26     0.04266         6   38    5    9     0.03802
       7   29    5    9    -0.03587         6   29    4    9    -0.03298
       7    9    5   23     0.03255         7   30    4    9     0.03214
       7    9    5   34    -0.03093         7   22    7    9     0.03022
       7   43    4    9    -0.03016
*****************************************************************************
Singlet       AU      ***********************************************************
###   1-st  ###           ---   7th state in this spin multiplicity ---
    Total energy       in au =     -77.988753
    Correlation energy in au =       0.062119
    Excitation energy  in au =       0.324041    in eV =       8.817613
  *SINGLE EXCITATION
       8   12     0.87691         8   22     0.42326
       8   33     0.04874
  *DOUBLE EXCITATION
       8   25    8   12    -0.08731         8   35    8   12     0.08176
       8   12    7   33    -0.06997         8   12    5   29    -0.06556
       8   12    6   32    -0.06227         8   12    4   31     0.06048
       8   12    5   23    -0.05595         8   12    5   34     0.05108
       8   12    7   37     0.04956         8   25    8   22    -0.03973
       8   35    8   22     0.03673         8   12    7   22    -0.03513
```

```
      8   12    4   24    -0.03456         8   22    7   33    -0.03247
      8   22    5   29    -0.03228
###   2-nd  ###           ---  18th state in this spin multiplicity ---
    Total energy       in au =     -77.940407
    Correlation energy in au =       0.110465
    Excitation energy  in au =       0.372388    in eV =      10.133194
  *SINGLE EXCITATION
      8   22     0.86909         8   12    -0.42679
      8   33     0.11009
  *DOUBLE EXCITATION
      8   25    8   22    -0.08269         8   35    8   22     0.07690
      8   22    7   33    -0.06677         8   22    5   29    -0.06537
      8   22    6   32    -0.06033         8   22    4   31     0.05951
      8   22    5   23    -0.05275         8   22    7   37     0.04852
      8   25    8   12     0.04371         8   35    8   12    -0.04105
      8   27    8   23     0.04069         8   22    5   34     0.04062
      8   22    7   22    -0.03648         8   12    7   33     0.03455
      8   22    4   24    -0.03312         8   12    5   29     0.03153
      8   12    6   32     0.03053
*************************************************************************
Singlet       B1U     ******************************************************
###   1-st  ###           ---   4th state in this spin multiplicity ---
    Total energy       in au =     -78.014826
    Correlation energy in au =       0.036046
    Excitation energy  in au =       0.297968    in eV =       8.108129
  *SINGLE EXCITATION
      8   18     0.80718         8   14     0.41742
      8   27    -0.34286         6   38     0.06718
      7   29    -0.06115         7   23     0.04689
      4   26     0.04544         6   30    -0.03954
      5   33     0.03347         7   34    -0.03256
  *DOUBLE EXCITATION
      8   36    8   35     0.05397         8   18    5   29    -0.05180
      8   25    8   18    -0.04242         8   25    8   14    -0.03892
      8   35    8   18     0.03877         8   35    8   14     0.03643
      8   18    7   33    -0.03286         8   18    6   32    -0.03231
      8   18    4   31     0.03210         8   14    7   33    -0.03031
      8   14    5   29    -0.03019
###   2-nd  ###           ---  11th state in this spin multiplicity ---
    Total energy       in au =     -77.975764
    Correlation energy in au =       0.075108
    Excitation energy  in au =       0.337031    in eV =       9.171075
  *SINGLE EXCITATION
      8   14     0.86100         8   27     0.34867
      8   18    -0.28924         6   38    -0.03827
      7   23    -0.03786         7   29     0.03086
  *DOUBLE EXCITATION
      8   25    8   14    -0.08974         8   35    8   14     0.08369
      8   14    7   33    -0.07011         8   14    5   29    -0.06437
```

```
      8   14    6   32    -0.06233         8   14    4   31     0.06019
      8   14    5   23    -0.05618         8   14    5   34     0.05131
      8   14    7   37     0.04926         8   14    7   22    -0.03501
      8   14    4   24    -0.03479         8   36    8   35    -0.03177
      8   17    8   14    -0.03122
*****************************************************************************
Singlet       B2U     ***************************************************
###   1-st  ###           ---  10th state in this spin multiplicity ---
    Total energy       in au =     -77.987719
    Correlation energy in au =       0.063153
    Excitation energy  in au =       0.325075    in eV =       8.845747
  *SINGLE EXCITATION
      8   15     0.87108         8   20     0.43916
  *DOUBLE EXCITATION
      8   25    8   15    -0.08833         8   35    8   15     0.08261
      8   15    7   33    -0.06949         8   15    5   29    -0.06353
      8   15    6   32    -0.06112         8   15    4   31     0.05912
      8   15    5   23    -0.05556         8   15    5   34     0.05126
      8   15    7   37     0.04812         8   25    8   20    -0.04754
      8   35    8   20     0.04295         8   15    7   22    -0.03432
      8   20    7   33    -0.03428         8   15    4   24    -0.03409
###   2-nd  ###           ---  17th state in this spin multiplicity ---
    Total energy       in au =     -77.943665
    Correlation energy in au =       0.107207
    Excitation energy  in au =       0.369130    in eV =      10.044534
  *SINGLE EXCITATION
      8   20     0.87126         8   15    -0.43908
  *DOUBLE EXCITATION
      8   25    8   20    -0.09379         8   35    8   20     0.08496
      8   20    7   33    -0.06801         8   20    5   29    -0.05999
      8   20    6   32    -0.05898         8   20    4   31     0.05699
      8   20    5   23    -0.05431         8   20    5   34     0.05169
      8   25    8   15     0.04347         8   35    8   15    -0.04126
      8   20    7   37     0.03870         8   15    7   33     0.03515
      8   20    4   24    -0.03306         8   15    5   29     0.03289
      8   20    7   22    -0.03247         8   15    6   32     0.03136
      8   20    8   17    -0.03039         8   15    4   31    -0.03032
*****************************************************************************
Singlet       B3U     ***************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    Total energy       in au =     -78.049801
    Correlation energy in au =       0.001071
    Excitation energy  in au =       0.262993    in eV =       7.156411
  *SINGLE EXCITATION
      8    9     0.87815         8   26     0.34057
      8   16     0.16628         8   19    -0.15150
      8   13     0.07471         8   28    -0.07424
      8   32     0.04009
  *DOUBLE EXCITATION
```

```
      8   25    8    9    -0.08910         8   35    8    9     0.08114
      8    9    7   33    -0.06583         8    9    5   29    -0.06279
      8    9    6   32    -0.05908         8    9    4   31     0.05793
      8    9    5   23    -0.05262         8   27    8   24     0.04574
      8    9    5   34     0.04192         8    9    7   37     0.03951
      8   26    8   25    -0.03454         8    9    4   24    -0.03233
      8    9    7   22    -0.03196         8   24    8   18    -0.03145
      8   17    8    9    -0.03021
###   2-nd  ###           ---   6th state in this spin multiplicity ---
    Total energy       in au =     -77.991699
    Correlation energy in au =       0.059173
    Excitation energy  in au =       0.321096    in eV =       8.737465
  *SINGLE EXCITATION
      8   13     0.75034         8   19     0.54814
      8   16     0.27064         8   28     0.10732
      8   21     0.06217         8   26    -0.03681
      8   32     0.03295
  *DOUBLE EXCITATION
      8   25    8   13    -0.07525         8   35    8   13     0.07055
      8   13    7   33    -0.05878         8   13    5   29    -0.05571
      8   13    6   32    -0.05396         8   25    8   19    -0.05337
      8   13    4   31     0.05208         8   35    8   19     0.05032
      8   13    5   23    -0.03845         8   13    5   34     0.03603
      8   13    7   37     0.03592         8   19    7   33    -0.03501
      8   19    5   29    -0.03244         8   19    4   31     0.03203
      8   19    6   32    -0.03145
###   3-rd  ###           ---   9th state in this spin multiplicity ---
    Total energy       in au =     -77.987998
    Correlation energy in au =       0.062874
    Excitation energy  in au =       0.324797    in eV =       8.838162
  *SINGLE EXCITATION
      8   16     0.78383         8   21    -0.47131
      8   13    -0.30428         8    9    -0.11708
      8   19     0.08128         8   32    -0.04301
  *DOUBLE EXCITATION
      8   25    8   16    -0.08180         8   35    8   16     0.07594
      8   16    7   33    -0.06130         8   16    5   29    -0.05631
      8   16    6   32    -0.05492         8   25    8   21     0.05376
      8   16    4   31     0.05264         8   16    5   23    -0.04868
      8   35    8   21    -0.04752         8   16    5   34     0.03836
      8   16    7   37     0.03613         8   21    7   33     0.03485
      8   21    5   29     0.03291         8   21    6   32     0.03202
      8   21    4   31    -0.03064         8   16    4   24    -0.03058
      8   16    7   22    -0.03036         8   25    8   13     0.03010
###   4-th  ###           ---  12th state in this spin multiplicity ---
    Total energy       in au =     -77.957194
    Correlation energy in au =       0.093678
    Excitation energy  in au =       0.355600    in eV =       9.676378
  *SINGLE EXCITATION
```

```
      8   19    -0.66846         8   13     0.46313
      8    9    -0.33194         8   26     0.32005
      8   28    -0.20766         8   16     0.19547
  *DOUBLE EXCITATION
      8   25    8   19     0.06398         8   35    8   19    -0.06069
      8   25    8   13    -0.04688         8   35    8   13     0.04391
      8   19    7   33     0.04194         8   19    5   29     0.03832
      8   19    4   31    -0.03791         8   19    6   32     0.03704
      8   13    7   33    -0.03666         8   25    8    9     0.03603
      8   13    5   29    -0.03370         8   19    5   34    -0.03324
      8   19    5   23     0.03281         8   13    6   32    -0.03273
      8   35    8    9    -0.03261         8   13    4   31     0.03150
###   5-th  ###           ---  15th state in this spin multiplicity ---
    Total energy       in au =     -77.945710
    Correlation energy in au =       0.105162
    Excitation energy  in au =       0.367085    in eV =       9.988879
  *SINGLE EXCITATION
      8   21    -0.82540         8   16    -0.44104
      8   13     0.18563         8   26     0.16185
      8   32    -0.09260         8   19     0.06381
      8   28     0.05021
  *DOUBLE EXCITATION
      8   25    8   21     0.09435         8   35    8   21    -0.08425
      8   21    7   33     0.06150         8   21    5   29     0.05754
      8   21    6   32     0.05620         8   21    4   31    -0.05383
      8   21    5   23     0.04856         8   25    8   16     0.04132
      8   35    8   16    -0.04022         8   21    5   34    -0.03865
      8   21    7   37    -0.03649         8   16    7   33     0.03529
      8   16    5   29     0.03348         8   16    6   32     0.03201
      8   16    4   31    -0.03092         8   21    4   24     0.03086
==============================================================
  STEP #DENS#  Density Calculation
==============================================================
Transition density for SAC/SAC-CI (V)
Threshold for S2 operators (CThreDensULS2):  0.50D-02
Threshold for R1,R2 operators (CThreDensULR1):  0.10D+00
Only right vectors are used. (ILEFT=0)
------------------------------------------------------------------------------
Transition dipole moment of   singlet state from SAC ground state
------------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
------------------------------------------------------------------------------
   AG         0      0.0          Excitations are from this state.
   AG         1      8.1554      0.0000      0.0000      0.0000      0.0000
   AG         2     10.4763      0.0000      0.0000      0.0000      0.0000
   B1G        1      7.7962      0.0000      0.0000      0.0000      0.0000
   B1G        2      8.8213      0.0000      0.0000      0.0000      0.0000
   B1G        3      9.9000      0.0000      0.0000      0.0000      0.0000
```

Transition dipole moments and oscillator strengths of the excited states.are summarized. SAC w.f. is used for the ground state.

```
   B2G        1      7.8207      0.0000      0.0000      0.0000      0.0000
   B2G        2     10.0407      0.0000      0.0000      0.0000      0.0000
   B2G        3     10.2314      0.0000      0.0000      0.0000      0.0000
   B3G        1      9.7442      0.0000      0.0000      0.0000      0.0000
   AU         1      8.8176      0.0000      0.0000      0.0000      0.0000
   AU         2     10.1332      0.0000      0.0000      0.0000      0.0000
   B1U        1      8.1081      0.0000      0.0000     -1.3552      0.3649
   B1U        2      9.1711      0.0000      0.0000      0.5260      0.0622
   B2U        1      8.8457      0.0000     -0.3057      0.0000      0.0202
   B2U        2     10.0445      0.0000     -0.4275      0.0000      0.0450
   B3U        1      7.1564     -0.6730      0.0000      0.0000      0.0794
   B3U        2      8.7375     -0.1437      0.0000      0.0000      0.0044
   B3U        3      8.8382     -0.4746      0.0000      0.0000      0.0488
   B3U        4      9.6764     -0.0351      0.0000      0.0000      0.0003
   B3U        5      9.9889     -0.6782      0.0000      0.0000      0.1126
-------------------------------------------------------------------------------
================================================================
  STEP #CIMX#  CI matrix elements          ### TRIPLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Triplet   AG    CONVERGED
Solution for Triplet   B1G   CONVERGED
Solution for Triplet   B2G   CONVERGED
Solution for Triplet   B3G   CONVERGED
Solution for Triplet   AU    CONVERGED
Solution for Triplet   B1U   CONVERGED
Solution for Triplet   B2U   CONVERGED
Solution for Triplet   B3U   CONVERGED
================================================================
  STEP #ULINTT#  Unlinked integral for Triplet State (SAC-CI)
================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
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  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Triplet   AG    CONVERGED
Solution for Triplet   B1G   CONVERGED
Solution for Triplet   B2G   CONVERGED
Solution for Triplet   B3G   CONVERGED
Solution for Triplet   AU    CONVERGED
Solution for Triplet   B1U   CONVERGED
Solution for Triplet   B2U   CONVERGED
```

Result of SAC-CI calculation for triplet state. Total energy, correlation energy (HF energy as the reference), excitation energy (SAC total energy as the reference), and the SAC-CI coefficients are shown. For example, the first excited state in triplet A_g symmetry is the triplet excitation from 8-th MO to 17-th MO, and its coefficient is 0.89. The excitation energy is 8.01 eV.

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Solution for Triplet   B3U   CONVERGED
**********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
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Triplet       AG      ***********************************************************
###   1-st  ###           ---   5th state in this spin multiplicity ---
    Total energy       in au =     -78.018557
    Correlation energy in au =       0.032316
    Excitation energy  in au =       0.294238    in eV =       8.006628
  *SINGLE EXCITATION
       8   17     0.88725         8   25     0.40530
       8   35    -0.06770
  *DOUBLE EXCITATION
       8   35    8   17     0.08406         8   25    8   17    -0.07473
       7   33    8   17    -0.06968         5   29    8   17    -0.06394
       6   32    8   17    -0.06057         4   31    8   17     0.05944
       5   23    8   17    -0.05431         5   34    8   17     0.05041
       7   37    8   17     0.04774         8   35    8   25     0.03754
       4   24    8   17    -0.03376         7   22    8   17    -0.03299
###   2-nd  ###           ---  20th state in this spin multiplicity ---
    Total energy       in au =     -77.936222
    Correlation energy in au =       0.114650
    Excitation energy  in au =       0.376573    in eV =      10.247061
  *SINGLE EXCITATION
       8   25     0.88055         8   17    -0.40624
       8   35    -0.13680
  *DOUBLE EXCITATION
       8   35    8   25     0.07885         8   25    8   17     0.07769
       7   33    8   25    -0.06109         6   32    8   25    -0.05666
       5   29    8   25    -0.05547         4   31    8   25     0.05379
       8   35    8   17    -0.04164         5   34    8   25     0.03717
       7   33    8   17     0.03558         7   37    8   25     0.03474
       5   29    8   17     0.03291         6   32    8   17     0.03079
       4   25    8   24     0.03012
*******************************************************************************
Triplet       B1G     ****************************************************
###   1-st  ###           ---   4th state in this spin multiplicity ---
    Total energy       in au =     -78.027144
    Correlation energy in au =       0.023728
    Excitation energy  in au =       0.285651    in eV =       7.772950
  *SINGLE EXCITATION
       8   11     0.84536         8   23     0.47061
       8   29     0.09579         8   34    -0.07652
       7   27     0.04197         7   18    -0.03721
  *DOUBLE EXCITATION
       8   25    8   11    -0.08179         8   35    8   11     0.07731
       7   33    8   11    -0.06666         5   29    8   11    -0.06112
       4   31    8   11     0.05738         6   32    8   11    -0.05732
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      5   23    8   11    -0.04474         5   34    8   11     0.04219
      7   37    8   11     0.03955         8   25    8   23    -0.03883
      8   35    8   23     0.03761         4   24    8   11    -0.03187
      7   33    8   23    -0.03167         7   22    8   11    -0.03070
###   2-nd  ###           ---   6th state in this spin multiplicity ---
    Total energy       in au =     -78.000013
    Correlation energy in au =       0.050859
    Excitation energy  in au =       0.312781    in eV =       8.511210
  *SINGLE EXCITATION
      7   18     0.70918         7   27    -0.63795
      7   14     0.13343         7   36    -0.11878
      8   11     0.07052
  *DOUBLE EXCITATION
      8   27    5   18    -0.10666         8   27    5   27     0.08956
      8   18    5   27    -0.07300         8   18    5   18     0.07187
      8   36    5   18    -0.03794         8   35    7   36     0.03629
      6   38    5   18    -0.03292
###   3-rd  ###           ---  16th state in this spin multiplicity ---
    Total energy       in au =     -77.950152
    Correlation energy in au =       0.100720
    Excitation energy  in au =       0.362643    in eV =       9.868018
  *SINGLE EXCITATION
      8   23    -0.81588         8   11     0.48211
      8   29    -0.20098         8   34     0.12806
      7   18    -0.03891
  *DOUBLE EXCITATION
      8   25    8   23     0.07164         8   35    8   23    -0.06820
      7   33    8   23     0.05632         8   25    8   11    -0.05200
      5   23    8   11    -0.04864         8   35    8   11     0.04831
      4   31    8   23    -0.04277         5   29    8   23     0.04158
      7   33    8   11    -0.04128         5   29    8   11    -0.03931
      6   32    8   23     0.03883         5   34    8   23    -0.03793
      6   32    8   11    -0.03729         4   31    8   11     0.03519
      7   37    8   23    -0.03490         8   33    8   27     0.03244
      8   23    5   23    -0.03161
*******************************************************************************
Triplet       B2G     ***************************************************
###   1-st  ###           ---   3rd state in this spin multiplicity ---
    Total energy       in au =     -78.027336
    Correlation energy in au =       0.023536
    Excitation energy  in au =       0.285458    in eV =       7.767717
  *SINGLE EXCITATION
      8   10    -0.86180         8   24    -0.43777
      8   31     0.11901
  *DOUBLE EXCITATION
      8   25    8   10     0.08318         8   35    8   10    -0.07866
      7   33    8   10     0.06736         5   29    8   10     0.06719
      6   32    8   10     0.06207         4   31    8   10    -0.06057
      5   23    8   10     0.05268         7   37    8   10    -0.04948
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      5   34    8   10    -0.04063         8   27    8   26    -0.03919
      8   25    8   24     0.03670         8   35    8   24    -0.03585
      5   29    8   24     0.03333         7   22    8   10     0.03144
      8   27    8    9    -0.03004
###   2-nd  ###          ---  13th state in this spin multiplicity ---
    Total energy       in au =     -77.959137
    Correlation energy in au =       0.091735
    Excitation energy  in au =       0.353658    in eV =       9.623523
  *SINGLE EXCITATION
      6   18    -0.67906         6   27     0.66774
      6   36     0.15863         6   14    -0.11538
      8   24    -0.05157         8   10     0.04567
      3   27    -0.04472
  *DOUBLE EXCITATION
      8   27    4   18     0.07502         8   27    4   27    -0.06730
      8   18    4   27     0.05418         8   18    4   18    -0.05226
      8   35    6   18    -0.03341         8   36    6   35    -0.03295
      8   35    6   36    -0.03260
###   3-rd  ###          ---  18th state in this spin multiplicity ---
    Total energy       in au =     -77.944624
    Correlation energy in au =       0.106248
    Excitation energy  in au =       0.368170    in eV =      10.018428
  *SINGLE EXCITATION
      8   24     0.83247         8   10    -0.45374
      8   31    -0.20928         6   27     0.05114
      6   18    -0.04612         8   40     0.04607
  *DOUBLE EXCITATION
      8   25    8   24    -0.07474         8   35    8   24     0.07194
      5   29    8   24    -0.06146         7   33    8   24    -0.05571
      8   27    8   26     0.05487         6   32    8   24    -0.05483
      4   31    8   24     0.05326         8   25    8   10     0.04882
      8   35    8   10    -0.04499         7   33    8   10     0.03993
      8   24    5   23     0.03825         7   37    8   24     0.03715
      5   24    8   23     0.03593         6   32    8   10     0.03569
      5   34    8   24     0.03563         5   29    8   10     0.03455
      4   31    8   10    -0.03399         8   23    5   24     0.03342
      5   23    8   10     0.03207         4   24    8   10     0.03121
*****************************************************************************
Triplet       B3G     ******************************************************
###   1-st  ###          ---  12th state in this spin multiplicity ---
    Total energy       in au =     -77.961651
    Correlation energy in au =       0.089221
    Excitation energy  in au =       0.351144    in eV =       9.555101
  *SINGLE EXCITATION
      7    9     0.84207         7   26     0.38187
      7   19    -0.18935         7   16     0.12179
      7   28    -0.11221         5   24     0.08327
      7   13     0.05932         7   32     0.05499
      4   23     0.05116         7   39     0.03357
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  *DOUBLE EXCITATION
      8   27    5    9    -0.12747         8   18    5    9     0.08696
      8   25    7    9    -0.06995         8   35    7    9     0.06989
      8   36    5    9    -0.06314         8   27    5   26    -0.04813
      7   33    7    9    -0.03912         6   38    5    9    -0.03610
      7   29    5    9     0.03327         5   27    8    9    -0.03194
      6   29    4    9     0.03157
*****************************************************************************
Triplet       AU      ************************************************************
###   1-st  ###           ---   9th state in this spin multiplicity ---
    Total energy       in au =     -77.988574
    Correlation energy in au =       0.062298
    Excitation energy  in au =       0.324221    in eV =       8.822501
  *SINGLE EXCITATION
      8   12     0.87347         8   22     0.43050
      8   33     0.05104
  *DOUBLE EXCITATION
      8   25    8   12    -0.08706         8   35    8   12     0.08168
      7   33    8   12    -0.06981         5   29    8   12    -0.06649
      6   32    8   12    -0.06195         4   31    8   12     0.06120
      5   23    8   12    -0.05618         5   34    8   12     0.05106
      7   37    8   12     0.05036         8   25    8   22    -0.04029
      8   35    8   22     0.03773         4   24    8   12    -0.03436
      7   33    8   22    -0.03349         5   29    8   22    -0.03349
      7   22    8   12    -0.03164         4   31    8   22     0.03054
###   2-nd  ###           ---  19th state in this spin multiplicity ---
    Total energy       in au =     -77.940788
    Correlation energy in au =       0.110084
    Excitation energy  in au =       0.372007    in eV =      10.122827
  *SINGLE EXCITATION
      8   22     0.86530         8   12    -0.43426
      8   33     0.11158
  *DOUBLE EXCITATION
      8   25    8   22    -0.08225         8   35    8   22     0.07715
      7   33    8   22    -0.06652         5   29    8   22    -0.06644
      4   31    8   22     0.06070         6   32    8   22    -0.05989
      5   23    8   22    -0.05347         5   34    8   22     0.05139
      7   37    8   22     0.05061         8   25    8   12     0.04461
      8   35    8   12    -0.04177         8   27    8   23     0.03746
      7   33    8   12     0.03520         5   29    8   12     0.03254
      4   24    8   22    -0.03200         6   32    8   12     0.03101
      4   31    8   12    -0.03016
*****************************************************************************
Triplet       B1U     ************************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    Total energy       in au =     -78.147373
    Correlation energy in au =      -0.096501
    Excitation energy  in au =       0.165422    in eV =       4.501360
  *SINGLE EXCITATION
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      8   27     0.69922         8   18    -0.66604
      8   36     0.17261         8   14    -0.11240
  *DOUBLE EXCITATION
      8   35    8   18    -0.03915         8   31    4   27     0.03784
      8   25    8   18     0.03447         8   35    8   27     0.03409
###   2-nd  ###           ---  11th state in this spin multiplicity ---
    Total energy       in au =     -77.983378
    Correlation energy in au =       0.067494
    Excitation energy  in au =       0.329417    in eV =       8.963888
  *SINGLE EXCITATION
      8   14     0.92652         8   27     0.26946
      8   18     0.13762         8   36     0.05053
  *DOUBLE EXCITATION
      8   25    8   14    -0.09306         8   35    8   14     0.08772
      7   33    8   14    -0.07563         5   29    8   14    -0.07042
      6   32    8   14    -0.06616         4   31    8   14     0.06479
      5   23    8   14    -0.05958         5   34    8   14     0.05428
      7   37    8   14     0.05317         7   22    8   14    -0.03680
      4   24    8   14    -0.03645
*************************************************************************
Triplet       B2U     ******************************************************
###   1-st  ###           ---  10th state in this spin multiplicity ---
    Total energy       in au =     -77.987852
    Correlation energy in au =       0.063020
    Excitation energy  in au =       0.324942    in eV =       8.842132
  *SINGLE EXCITATION
      8   15     0.85881         8   20     0.46363
  *DOUBLE EXCITATION
      8   25    8   15    -0.08681         8   35    8   15     0.08168
      7   33    8   15    -0.06982         5   29    8   15    -0.06387
      6   32    8   15    -0.06015         4   31    8   15     0.05907
      5   23    8   15    -0.05516         5   34    8   15     0.05053
      7   37    8   15     0.04847         8   35    8   20     0.04409
      8   25    8   20    -0.04401         7   33    8   20    -0.03662
      7   22    8   15    -0.03348         4   24    8   15    -0.03329
      5   29    8   20    -0.03297         6   32    8   20    -0.03104
      4   31    8   20     0.03051
###   2-nd  ###           ---  17th state in this spin multiplicity ---
    Total energy       in au =     -77.945239
    Correlation energy in au =       0.105633
    Excitation energy  in au =       0.367555    in eV =      10.001686
  *SINGLE EXCITATION
      8   20     0.85933         8   15    -0.46320
  *DOUBLE EXCITATION
      8   25    8   20    -0.08113         8   35    8   20     0.08111
      7   33    8   20    -0.06792         5   29    8   20    -0.06213
      6   32    8   20    -0.05829         4   31    8   20     0.05724
      5   23    8   20    -0.05166         5   34    8   20     0.05080
      8   25    8   15     0.04736         7   37    8   20     0.04703
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      8   35    8   15    -0.04380         7   33    8   15     0.03784
      5   29    8   15     0.03519         6   32    8   15     0.03297
      4   31    8   15    -0.03237         4   24    8   20    -0.03204
      7   22    8   20    -0.03149         5   23    8   15     0.03014
*************************************************************************
Triplet       B3U     ******************************************************
###   1-st  ###           ---   2nd state in this spin multiplicity ---
    Total energy       in au =     -78.053125
    Correlation energy in au =      -0.002253
    Excitation energy  in au =       0.259670    in eV =       7.065972
  *SINGLE EXCITATION
      8    9     0.86123         8   26     0.38342
      8   16     0.17219         8   19    -0.15168
      8   28    -0.07278         8   13     0.06954
      8   21    -0.04826         8   39     0.03234
  *DOUBLE EXCITATION
      8   25    8    9    -0.07854         8   35    8    9     0.07769
      7   33    8    9    -0.06462         5   29    8    9    -0.06258
      6   32    8    9    -0.06002         4   31    8    9     0.05902
      5   34    8    9     0.03997         7   37    8    9     0.03918
      5   23    8    9    -0.03855         4   24    8    9    -0.03218
      8   27    8   24     0.03167
###   2-nd  ###           ---   7th state in this spin multiplicity ---
    Total energy       in au =     -77.991295
    Correlation energy in au =       0.059577
    Excitation energy  in au =       0.321500    in eV =       8.748452
  *SINGLE EXCITATION
      8   13     0.69114         8   19     0.57317
      8   16     0.36268         8   28     0.12968
  *DOUBLE EXCITATION
      8   25    8   13    -0.06926         8   35    8   13     0.06517
      8   25    8   19    -0.05425         7   33    8   13    -0.05406
      8   35    8   19     0.05241         5   29    8   13    -0.05200
      6   32    8   13    -0.04937         4   31    8   13     0.04080
      8   25    8   16    -0.03706         8   35    8   16     0.03529
      7   33    8   19    -0.03508         5   23    8   13    -0.03499
      5   29    8   19    -0.03442         5   34    8   13     0.03307
      7   37    8   13     0.03301         4   31    8   19     0.03264
      6   32    8   19    -0.03249
###   3-rd  ###           ---   8th state in this spin multiplicity ---
    Total energy       in au =     -77.988640
    Correlation energy in au =       0.062232
    Excitation energy  in au =       0.324155    in eV =       8.820708
  *SINGLE EXCITATION
      8   16     0.68879         8   21    -0.53161
      8   13    -0.40123         8    9    -0.15798
      8   32    -0.07919         8   26     0.07739
      8   28     0.03841
  *DOUBLE EXCITATION
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      8   25    8   16    -0.06953         8   35    8   16     0.06639
      7   33    8   16    -0.05368         5   29    8   16    -0.04983
      8   35    8   21    -0.04891         6   32    8   16    -0.04784
      8   25    8   21     0.04713         8   25    8   13     0.04020
      7   33    8   21     0.03953         4   31    8   16     0.03927
      8   35    8   13    -0.03755         5   23    8   16    -0.03472
      5   34    8   16     0.03321         7   37    8   16     0.03171
      7   33    8   13     0.03128         5   29    8   13     0.03093
      5   29    8   21     0.03031
###   4-th  ###           ---  14th state in this spin multiplicity ---
    Total energy       in au =     -77.958104
    Correlation energy in au =       0.092768
    Excitation energy  in au =       0.354691    in eV =       9.651628
  *SINGLE EXCITATION
      8   19     0.61479         8   13    -0.48909
      8   26    -0.38158         8    9     0.36122
      8   28     0.20386         8   16    -0.12503
      8   21     0.07629         8   32     0.03048
  *DOUBLE EXCITATION
      8   25    8   19    -0.05788         8   35    8   19     0.05610
      8   25    8   13     0.04973         8   35    8   13    -0.04659
      8   25    8    9    -0.04110         7   33    8   13     0.03873
      8   35    8    9     0.03772         5   29    8   19    -0.03621
      5   29    8   13     0.03603         7   33    8   19    -0.03566
      6   32    8   13     0.03458         4   31    8   19     0.03445
      6   32    8   19    -0.03401         7   33    8    9    -0.03200
###   5-th  ###           ---  15th state in this spin multiplicity ---
    Total energy       in au =     -77.950429
    Correlation energy in au =       0.100443
    Excitation energy  in au =       0.362366    in eV =       9.860472
  *SINGLE EXCITATION
      8   21    -0.71594         8   16    -0.55085
      8   26     0.26857         8   19     0.19221
      8   32    -0.11746         8   28     0.10776
      8   13     0.09423
  *DOUBLE EXCITATION
      8   35    8   21    -0.06472         8   25    8   21     0.06129
      8   25    8   16     0.05894         7   33    8   21     0.05343
      8   35    8   16    -0.05318         7   33    8   16     0.04375
      5   29    8   16     0.04174         5   29    8   21     0.03961
      6   32    8   16     0.03944         6   32    8   21     0.03892
      4   31    8   21    -0.03882         5   34    8   21    -0.03326
      5   23    8   21     0.03309         4   31    8   16    -0.03271
      7   37    8   21    -0.03036
================================================================
  STEP #DENS#  Density Calculation
================================================================
Transition density for SAC/SAC-CI (V)
Threshold for S2 operators (CThreDensULS2):  0.50D-02
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Transition dipole moments and oscillator strengths of the triplet excited states are summarized. The lowest state in the triplet symmetry is used for the ground state.

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Threshold for R1,R2 operators (CThreDensULR1):  0.10D+00
Left and right vectors are used. (ILEFT=1)
-------------------------------------------------------------------------------
Transition dipole moment of   triplet state from symmetry B1U    1-th state
-------------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
-------------------------------------------------------------------------------
   AG         1      3.5053      0.0000      0.0000      0.4715      0.0191
   AG         2      5.7457      0.0000      0.0000      0.2080      0.0061
   B1G        1      3.2716      0.0000      0.0000      0.0000      0.0000
   B1G        2      4.0099      0.0000      0.0000      0.0000      0.0000
   B1G        3      5.3667      0.0000      0.0000      0.0000      0.0000
   B2G        1      3.2664     -0.5774      0.0000      0.0000      0.0267
   B2G        2      5.1222      0.1184      0.0000      0.0000      0.0018
   B2G        3      5.5171      0.3273      0.0000      0.0000      0.0145
   B3G        1      5.0537      0.0000     -0.0120      0.0000      0.0000
   AU         1      4.3211      0.0000      0.0000      0.0000      0.0000
   AU         2      5.6215      0.0000      0.0000      0.0000      0.0000
   B1U        1      0.0          Excitations are from this state.
   B1U        2      4.4625      0.0000      0.0000      0.0000      0.0000
   B2U        1      4.3408      0.0000      0.0000      0.0000      0.0000
   B2U        2      5.5003      0.0000      0.0000      0.0000      0.0000
   B3U        1      2.5646      0.0000      0.0000      0.0000      0.0000
   B3U        2      4.2471      0.0000      0.0000      0.0000      0.0000
   B3U        3      4.3193      0.0000      0.0000      0.0000      0.0000
   B3U        4      5.1503      0.0000      0.0000      0.0000      0.0000
   B3U        5      5.3591      0.0000      0.0000      0.0000      0.0000
-------------------------------------------------------------------------------
================================================================
  STEP #CIMX#  CI matrix elements          ### IONIZED STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Ionized   AG    CONVERGED
Solution for Ionized   B3G   CONVERGED
Solution for Ionized   B1U   CONVERGED
Solution for Ionized   B2U   CONVERGED
Solution for Ionized   B3U   CONVERGED
================================================================
  STEP #ULINTIA#  Unlinked integral for Ionized State (SAC-CI)
================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
================================================================
  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
```

```
=============================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Ionized   AG    CONVERGED
Solution for Ionized   B3G   CONVERGED
Solution for Ionized   B1U   CONVERGED
Solution for Ionized   B2U   CONVERGED
Solution for Ionized   B3U   CONVERGED
***********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
***********************************************
*****************************************************************************
CationDoublet AG      ****************************************************
###   1-st  ###           ---   3rd state in this spin multiplicity ---
    Total energy       in au =     -77.777387
    Correlation energy in au =       0.273485
    Excitation energy  in au =       0.535408    in eV =      14.569191
  *SINGLE EXCITATION
       6     0.96053
  *DOUBLE EXCITATION
       8   35    6     0.10523         8   27    4    -0.09983
       8   25    6    -0.09382         7   33    6    -0.07686
       6   32    6    -0.07482         8   18    4     0.06938
       5   34    6     0.06445         5   23    6    -0.06001
       5   29    6    -0.04736         8   36    4    -0.04579
       6   38    4    -0.04154         7   29    4     0.04084
       4   31    6     0.04014         7   28    7    -0.03806
       4   24    6    -0.03799         7   22    6    -0.03624
       5   29    3     0.03613         8   45    3     0.03586
       3   39    6    -0.03341         6   26    6    -0.03316
       8   17    6    -0.03046         6   32    3     0.03038
###   2-nd  ###           ---   6th state in this spin multiplicity ---
    Total energy       in au =     -77.422325
    Correlation energy in au =       0.628547
    Excitation energy  in au =       0.890470    in eV =      24.230922
  *SINGLE EXCITATION
       3     0.85430
  *DOUBLE EXCITATION
       8   27    4    -0.30307         4   27    8    -0.25032
       8   18    4     0.21523         8   28    8     0.19004
       4   18    8     0.17722         8   32    8    -0.13680
       8   36    4    -0.13636         8   35    3     0.11262
       4   36    8    -0.11078         8   19    8     0.09797
       8   25    3    -0.09606         8    9    8    -0.09088
       8   26    8    -0.08598         8   21    8    -0.08360
       5   29    6     0.08065         6   29    5     0.07887
       7   33    3    -0.07703         7   28    7    -0.07553
       5   29    3    -0.07550         8   45    6     0.07342
       6   32    3    -0.07257         7   30    5    -0.06944
```

Result of SAC-CI calculation for ionized (cation doublet) state. Total energy, correlation energy (HF energy as the reference), ionization potential (SAC total energy as the reference), and the SAC-CI coefficients are shown. For example, the first ionized state in A_g symmetry is the ionization from 6-th MO, and its ionization energy is 14.57 eV.

```
      4   31    3     0.06736         5   34    3     0.06150
      6   32    6     0.06113         5   23    3    -0.05962
      6   45    8     0.05846         8   44    5     0.05584
      8   42    8     0.05173         8   50    8     0.04899
      6   38    4    -0.04332         6   41    5    -0.04322
      7   37    3     0.04227         5   41    6    -0.04180
      8   47    7     0.04005         5   44    8     0.03925
      5   28    5    -0.03811         7   37    6    -0.03782
      5   30    7    -0.03760         7   42    7    -0.03759
      4   38    6    -0.03625         7   33    6     0.03615
      4   24    3    -0.03577         4   40    3    -0.03526
      7   43    5     0.03508         3   35    8     0.03411
      7   47    8     0.03400         7   22    3    -0.03370
      5   23    6     0.03353         5   34    6    -0.03195
      8   17    3    -0.03053         7   46    6     0.03001
*****************************************************************************
CationDoublet B3G     ****************************************************
###   1-st  ###           ---   2nd state in this spin multiplicity ---
    Total energy       in au =     -77.839398
    Correlation energy in au =       0.211474
    Excitation energy  in au =       0.473396    in eV =      12.881771
  *SINGLE EXCITATION
      7     0.96508
  *DOUBLE EXCITATION
      8   27    5    -0.13740         8   18    5     0.09442
      8   25    7    -0.07997         8   35    7     0.07858
      8   36    5    -0.06843         7   33    7    -0.05737
      6   38    5    -0.05188         7   29    5     0.05121
      5   23    7    -0.03753         6   29    4     0.03697
      7   30    4    -0.03563         5   34    7     0.03485
      7   22    7    -0.03365         7   41    5    -0.03352
      7   43    4     0.03312         8   44    4     0.03180
      5   27    8    -0.03165         4   24    7    -0.03028
*****************************************************************************
CationDoublet B1U     ****************************************************
###   1-st  ###           ---   5th state in this spin multiplicity ---
    Total energy       in au =     -77.600774
    Correlation energy in au =       0.450098
    Excitation energy  in au =       0.712020    in eV =      19.375057
  *SINGLE EXCITATION
      4     0.92236
  *DOUBLE EXCITATION
      8   27    6    -0.22722         8   18    6     0.16557
      8   27    3    -0.12369         6   27    8    -0.09292
      8   36    6    -0.09122         8   35    4     0.09070
      8   25    4    -0.08508         8   18    3     0.08493
      7   30    7    -0.08378         6   29    7     0.07866
      8   31    8     0.07769         7   29    6     0.07591
      6   18    8     0.06805         8   36    3    -0.06452
```

```
      5   28    7    -0.06243         7   33    4    -0.06182
      3   27    8    -0.06101         6   38    6    -0.05876
      7   43    7     0.05450         7   28    5    -0.04825
      6   41    7    -0.04192         5   34    4     0.03904
      8   45    4     0.03903         3   18    8     0.03858
      7   41    6    -0.03828         6   38    3    -0.03795
      5   42    7    -0.03792         7   42    5    -0.03779
      6   26    4    -0.03766         5   23    4    -0.03700
      4   24    4    -0.03631         6   32    4    -0.03418
      4   31    4     0.03336         7   22    4    -0.03228
      6   36    8    -0.03211         4   38    4    -0.03208
      8   38    8     0.03171         3   36    8    -0.03170
      8   47    5     0.03151         8   44    7     0.03148
*****************************************************************************
CationDoublet B2U     ******************************************************
###   1-st  ###           ---   4th state in this spin multiplicity ---
    Total energy       in au =     -77.722818
    Correlation energy in au =       0.328054
    Excitation energy  in au =       0.589977    in eV =      16.054080
  *SINGLE EXCITATION
      5     0.94044
  *DOUBLE EXCITATION
      8   27    7    -0.22980         8   18    7     0.16497
      8   36    7    -0.10093         8   35    5     0.08835
      8   25    5    -0.08697         7   27    8    -0.07391
      7   29    7     0.06467         7   33    5    -0.06404
      7   18    8     0.05255         5   23    5    -0.05229
      6   38    7    -0.04249         5   29    5    -0.04089
      5   34    5     0.03887         7   41    7    -0.03723
      6   32    5    -0.03606         7   22    5    -0.03501
      4   31    5     0.03393         8   44    3     0.03233
      7   36    8    -0.03165         4   24    5    -0.03155
*****************************************************************************
CationDoublet B3U     ******************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    Total energy       in au =     -77.934386
    Correlation energy in au =       0.116486
    Excitation energy  in au =       0.378409    in eV =      10.297024
  *SINGLE EXCITATION
      8     0.97508
  *DOUBLE EXCITATION
      8   25    8    -0.09809         8   35    8     0.09193
      7   33    8    -0.07843         5   29    8    -0.07224
      6   32    8    -0.06910         4   31    8     0.06683
      5   23    8    -0.06231         5   34    8     0.05709
      7   37    8     0.05484         7   22    8    -0.04806
      4   24    8    -0.03847         8   17    8    -0.03286
      4   27    3    -0.03011
=============================================================
```

```
  STEP #SATEI#  Monopole Intensity Calculation
==============================================================
Symmetry  State     I.P.        Intensity
-------------------------------------------
AG          1      14.569       0.92274
            2      24.231       0.72985
-------------------------------------------
B3G         1      12.882       0.93138
-------------------------------------------
B1U         1      19.375       0.85074
-------------------------------------------
B2U         1      16.054       0.88443
-------------------------------------------
B3U         1      10.297       0.95078
-------------------------------------------
==============================================================
```

Monopole intensity for the ionizations. This is approximated intensity for the ionization spectrum.

```
  STEP #DENS#  Density Calculation
==============================================================
Transition density for SAC/SAC-CI (V)
Threshold for S2 operators (CThreDensULS2):  0.50D-02
Threshold for R1,R2 operators (CThreDensULR1):  0.10D+00
Left and right vectors are used. (ILEFT=1)
-----------------------------------------------------------------------------
Transition dipole moment of   ionized state from symmetry B3U    1-th state
-----------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
-----------------------------------------------------------------------------
   AG         1      4.2722      0.1149      0.0000      0.0000      0.0014
   AG         2     13.9339      0.3948      0.0000      0.0000      0.0532
   B3G        1      2.5847      0.0000      0.0000      0.0000      0.0000
   B1U        1      9.0780      0.0000      0.0000      0.0000      0.0000
   B2U        1      5.7571      0.0000      0.0000      0.0000      0.0000
   B3U        1      0.0          Excitations are from this state.
-----------------------------------------------------------------------------
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.

*********************************************************************

           Population analysis using the SCF density.

*********************************************************************

Orbital symmetries:
      Occupied  (AG) (B1U) (AG) (B1U) (B2U) (AG) (B3G) (B3U)
      Virtual   (AG) (B1U) (B2U) (B3G) (AG) (B2G) (B1G) (AG) (B3U)
                (B2G) (AG) (B1G) (AG) (B3G) (B2U) (B1U) (B3U)
                (AG) (B2G) (AG) (B2U) (B1U) (B1U) (AG) (B3G) (B2U)
```

Transition dipole moments and oscillator strengths of the ionized (cation doublet) states are summarized. The lowest ionized state is used for the ground state.

```
                (B3U) (B2G) (B3G) (B1U) (AG) (B1U) (B2U) (AG)
                (B1U) (B1G) (B3U) (B3G) (AU) (AG) (B3G) (AG) (B2U)
                (B1U) (B2G) (B2U) (B3U) (B1G) (B1U) (B2G) (AU)
                (AG) (B3G) (B1U) (AG) (B2U) (B1U) (B3G) (AG) (B1U)
The electronic state is 1-AG.
Alpha  occ. eigenvalues --  -11.24168 -11.24006  -1.03312  -0.79239  -0.64303
Alpha  occ. eigenvalues --   -0.58530  -0.50819  -0.37482
Alpha virt. eigenvalues --    0.03169   0.03468   0.03508   0.03551   0.03554
Alpha virt. eigenvalues --    0.03594   0.03658   0.03681   0.03845   0.10243
Alpha virt. eigenvalues --    0.11738   0.12373   0.12463   0.12670   0.15159
Alpha virt. eigenvalues --    0.15506   0.16761   0.18701   0.19263   0.36642
Alpha virt. eigenvalues --    0.36675   0.39651   0.42002   0.50170   0.56519
Alpha virt. eigenvalues --    0.63239   0.67847   0.68330   0.69338   0.87168
Alpha virt. eigenvalues --    0.96023   1.13895   1.20076   1.32574   1.33696
Alpha virt. eigenvalues --    1.53533   1.56517   1.60212   1.67370   1.96825
Alpha virt. eigenvalues --    2.07478   2.10752   2.11875   2.22033   2.24784
Alpha virt. eigenvalues --    2.43427   2.48609   2.56965   2.61687   2.78096
Alpha virt. eigenvalues --    2.84691   2.94824   2.99706   3.21255   3.36390
Alpha virt. eigenvalues --    3.51834   3.70422   3.93431  24.04900  24.38610
         Condensed to atoms (all electrons):
              1          2          3          4          5          6
    1  H    0.527370   0.412861  -0.038682  -0.005602   0.002285  -0.030002
    2  C    0.412861   4.861946   0.619506  -0.038682  -0.038682   0.412861
    3  C   -0.038682   0.619506   4.861946   0.412861   0.412861  -0.038682
    4  H   -0.005602  -0.038682   0.412861   0.527370  -0.030002   0.002285
    5  H    0.002285  -0.038682   0.412861  -0.030002   0.527370  -0.005602
    6  H   -0.030002   0.412861  -0.038682   0.002285  -0.005602   0.527370
    7  Bq   0.006713   0.002089   0.002089   0.006713   0.006713   0.006713
              7
    1  H    0.006713
    2  C    0.002089
    3  C    0.002089
    4  H    0.006713
    5  H    0.006713
    6  H    0.006713
    7  Bq   0.005399
Mulliken atomic charges:
              1
    1  H    0.125057
    2  C   -0.231900
    3  C   -0.231900
    4  H    0.125057
    5  H    0.125057
    6  H    0.125057
    7  Bq  -0.036428
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
              1
    1  H    0.000000
```

```
    2  C    0.018214
    3  C    0.018214
    4  H    0.000000
    5  H    0.000000
    6  H    0.000000
    7  Bq  -0.036428
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    83.5302
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     0.0000    Y=     0.0000    Z=     0.0000  Tot=     0.0000
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=   -16.2640   YY=   -12.2863   ZZ=   -12.1376
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -2.7013   YY=     1.2763   ZZ=     1.4250
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=     0.0000  YYY=     0.0000  ZZZ=     0.0000  XYY=     0.0000
 XXY=     0.0000  XXZ=     0.0000  XZZ=     0.0000  YZZ=     0.0000
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=   -21.6535 YYYY=   -27.0739 ZZZZ=   -68.5119 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=    -8.8502 XXZZ=   -16.1757 YYZZ=   -13.1232
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 3.324999423628D+01 E-N=-2.476162242765D+02  KE= 7.785168423628D+01
Symmetry AG   KE= 3.748532068494D+01
Symmetry B1G  KE= 9.684633491136D-34
Symmetry B2G  KE= 3.251299784892D-32
Symmetry B3G  KE= 2.083198795373D+00
Symmetry AU   KE= 1.257391018236D-33
Symmetry B1U  KE= 3.454340302188D+01
Symmetry B2U  KE= 1.827961283940D+00
Symmetry B3U  KE= 1.911800450144D+00

Test job not archived.
1¥1¥GINC-MIRAI86¥SP¥RSACCI¥Gen¥C2H4N1¥MASAHIRO¥31-Jul-2004¥0¥¥# SAC-CI
(LEVELONE, SINGLET=(NSTATE=(2,3,3,1,2,2,2,5)), TRIPLET=(NSTATE=(2,3,3,
1,2,2,2,5)), CATIONDOUBLET=(NSTATE=(2,0,0,1,0,1,1,1))) /GEN MASSAGE SY
MM=ON TEST¥¥Gaussian Test Job 635 (Part 1): Comparison of LevelOne, Le
velTwo, and LevelThree calculations for ethylene. First is LevelOne ca
lculation. SAC-CI SD-R calculations for singlet, triplet, and ionized
states of ethylene using Huzinaga-Dunning basis with polarization func
tions [4s2p1d/2s1p] plus Rydberg functions [2s2p2d] on center of molec
ule. Inner-shells are excluded from the active space and full-valence
active MOs are used (FC; default). Dummy atom is used with symmetry (M
assage,Symm=On). The results are summarized in Part I-L of the SAC-CI
Guide.¥¥0,1¥H¥C,1,1.0868¥C,2,1.3391,1,121.28¥H,3,1.0868,2,121.28,1,0.,
```

O¥H,3,1.0868,2,121.28,1,180.,O¥H,2,1.0868,3,121.28,4,180.,O¥Bq,2,0.669
55,1,121.28,4,0.,O¥¥Version=AI64T-G03RevC.02¥State=1-AG¥HF=-78.050872¥
RMSD=3.635e-09¥PG=D02H [O(N1),C2"(C1.C1),SG(H4)]¥¥@

YOU CAN WIPE THE SLATE CLEAN, BUT YOU'LL STILL
HAVE TO EAT A LITTLE CHALK DUST.

```
Job cpu time:  0 days  0 hours  3 minutes 27.4 seconds.
File lengths (MBytes):  RWF=    553 Int=      0 D2E=      0 Chk=     13 Scr=     48
Normal termination of Gaussian 03 at Sat Jul 31 11:52:03 2004.
Initial command:
/work/g03.C02/g03/l1.exe /work/g03.C02/inputs/Gau-113434.inp -scrdir=/work/g03.C02/inputs/
Entering Link 1 = /work/g03.C02/g03/l1.exe PID=    113452.
```

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H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
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A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
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C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

****************************************
Gaussian 03:  AI64T-G03RevC.02 12-Jun-2004
               31-Jul-2004
****************************************
%mem=12mw
---------------------------------------------------------------------------
# SAC-CI(LevelTwo, Singlet=(NState=(2,3,3,1,2,2,2,5)), Triplet=(NState
=(2,3,3,1,2,2,2,5)), CationDoublet=(NState=(2,0,0,1,0,1,1,1))) /Gen Ma
ssage Symm=On test
---------------------------------------------------------------------------
1/38=1/1;
2/15=-1,17=6,18=5,40=1/2;
3/5=7,10=10,11=9,16=1,25=1,30=1,36=2/1,2,3;
4//1;
```

This calculation requires LevelTwo accuracy in the perturbation selection. The result is compared with that with “LevelOne” and “LevelThree” results. See secton I-L for the detailed descriptions.

```
5/5=2,38=5/2;
8/6=5,9=30000,10=1,40=1,42=2/1,4;
9//23;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;
-----------------------------------------------------------------------
Gaussian Test Job 635 (Part 2): SAC-CI SD-R LevelTwo calculations for
ethylene.
-----------------------------------------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
H1
C2                  1    r1
C3                  2    r2       1    a1
H4                  3    r1       2    a1       1     0.       0
H5                  3    r1       2    a1       1     180.     0
H6                  2    r1       3    a1       4     180.     0
N7                  2    r22      1    a1       4     0.       0
      Variables:
 r1                   1.0868
 r2                   1.3391
 a1                 121.28
 r22                  0.66955

                        Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          1           0        0.000000    0.000000    0.000000
   2          6           0        0.000000    0.000000    1.086800
   3          6           0        1.144449    0.000000    1.782089
   4          1           0        2.108977    0.000000    1.281270
   5          1           0        1.144449    0.000000    2.868889
   6          1           0       -0.964528    0.000000    1.587619
   7          7           0        0.572224    0.000000    1.434444
---------------------------------------------------------------------
                    Distance matrix (angstroms):
                    1          2          3          4          5
    1  H    0.000000
    2  C    1.086800   0.000000
    3  C    2.117924   1.339100   0.000000
    4  H    2.467678   2.117924   1.086800   0.000000
    5  H    3.088735   2.117924   1.086800   1.857646   0.000000
    6  H    1.857646   1.086800   2.117924   3.088735   2.467678
    7  N    1.544368   0.669550   0.669550   1.544368   1.544368
                    6          7
    6  H    0.000000
    7  N    1.544368   0.000000
```

```
Stoichiometry    C2H4N
Framework group  D2H[O(N),C2"(C.C),SG(H4)]
Deg. of freedom     3
Full point group                 D2H     NOp   8
Largest Abelian subgroup         D2H     NOp   8
Largest concise Abelian subgroup D2      NOp   4
                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          1            0        0.000000    0.928823    1.233839
   2          6            0        0.000000    0.000000    0.669550
   3          6            0        0.000000    0.000000   -0.669550
   4          1            0        0.000000    0.928823   -1.233839
   5          1            0        0.000000   -0.928823   -1.233839
   6          1            0        0.000000   -0.928823    1.233839
   7          7            0        0.000000    0.000000    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    145.3135944     29.9107742     24.8050094
General basis read from cards:  (5D, 7F)
The nuclear charge for atom    7 has been changed to Z=  0   0.000000
There are    18 symmetry adapted basis functions of AG  symmetry.
There are     4 symmetry adapted basis functions of B1G symmetry.
There are     6 symmetry adapted basis functions of B2G symmetry.
There are     9 symmetry adapted basis functions of B3G symmetry.
There are     2 symmetry adapted basis functions of AU  symmetry.
There are    14 symmetry adapted basis functions of B1U symmetry.
There are     9 symmetry adapted basis functions of B2U symmetry.
There are     6 symmetry adapted basis functions of B3U symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   68 basis functions,   108 primitive gaussians,    72 cartesian basis functions
    8 alpha electrons        8 beta electrons
      nuclear repulsion energy        33.2499942363 Hartrees.
NAtoms=    7 NActive=    7 NUniq=    3 SFac= 5.66D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    68 RedAO= T  NBF=    18     4     6     9     2    14     9     6
NBsUse=    68 1.00D-06 NBFU=    18     4     6     9     2    14     9     6
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.13D-02 ExpMax= 4.23D+03 ExpMxC= 6.35D+02 IAcc=3 IRadAn=         5 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=         5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Warning:  off-atom basis functions, so minimal bfn integration tests in XC quadrature.
Initial guess orbital symmetries:
      Occupied  (AG) (B1U) (AG) (B1U) (B2U) (AG) (B3G) (B3U)
      Virtual   (B2G) (AG) (B2U) (B1U) (B3U) (AG) (B3G) (AG) (B2G)
                (B1G) (AG) (B2U) (B1U) (B3G) (AG) (B1G) (AG) (B3U)
```

```
                (B2G) (B2U) (B1U) (AG) (B1U) (AG) (B3G) (B2U)
                (B2G) (B3U) (B1U) (B3G) (AG) (B1U) (B2U) (AG)
                (B1U) (B1G) (B3U) (B3G) (AU) (AG) (AG) (B3G) (B2U)
                (B1U) (B2G) (B2U) (B3U) (B1U) (B1G) (B2G) (AU)
                (AG) (B3G) (B1U) (AG) (B2U) (B1U) (B3G) (AG) (B1U)
The electronic state of the initial guess is 1-AG.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=     4505542.
SCF Done:  E(RHF) =  -78.0508720221     A.U. after    9 cycles
            Convg  =    0.3635D-08             -V/T =  2.0026
            S**2   =   0.0000
ExpMin= 1.13D-02 ExpMax= 4.23D+03 ExpMxC= 6.35D+02 IAcc=3 IRadAn=         5 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=         5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Warning:  off-atom basis functions, so minimal bfn integration tests in XC quadrature.
Range of M.O.s used for correlation:     3    68
NBasis=    68 NAE=     8 NBE=     8 NFC=     2 NFV=     0
NROrb=     66 NOA=     6 NOB=     6 NVA=    60 NVB=    60
--------------------------------------------------------------------
####################################################################
--------------------------------------------------------------------
              SAC/SAC-CI Program Combined with GAUSSIAN
                            for Calculating
        Ground, Excited, Ionized, and Electron-Attached States
                                and
             Singlet, Doublet, Triplet, Quartet, Quintet,
                   Sextet, and Septet Spin States
                                and
                  Their Analytical Energy Gradients
                         coded originally by
                          Hiroshi Nakatsuji
                           and extended by
 H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa,
       M. Ishida, T. Nakajima, Y. Honda, O. Kitao, and H. Nakai
                                at
                 Department of Hydrocarbon Chemistry,
                Division of Molecular Engineering, and
      Department of Synthetic Chemistry & Biological Chemistry,
                   Graduate School of Engineering,
                         Kyoto University,
                       Kyoto 606-8501, Japan
--------------------------------------------------------------------
####################################################################
--------------------------------------------------------------------
No. of INTEGRALS =    324236 NBLK =       202 KOUNT =      1036
##############################################################################
```

```
    Singles-Doubles (SD) SAC/SAC-CI  (SAC-CI SD-R)
##############################################################################
==============================================================
  STEP #PRES#  Generation of Linked Operators and Selection
==============================================================
== States to be calculated ==
           AG   B1G  B2G  B3G  AU   B1U  B2U  B3U
SINGLET    Yes  Yes  Yes  Yes  Yes  Yes  Yes  Yes
TRIPLET    Yes  Yes  Yes  Yes  Yes  Yes  Yes  Yes
IONIZED    Yes  Yes  Yes  Yes  Yes  Yes  Yes  Yes
ANIONIZED  No   No   No   No   No   No   No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  3,  3,  3,  1,  2,  2,  2,  5)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelTwo #
  EThreS2 (Lambda_G)=  0.500D-05(au)   EThreR2 (Lambda_E)=  0.500D-06(au)
TRIPLET STATE
 Number of States  Triplet      =(  2,  3,  3,  1,  2,  2,  2,  5)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelTwo #
  EThreR2 (Lambda_E)=  0.500D-06(au)
IONIZED STATE
 Number of States  CationDoublet=(  2,  0,  0,  1,  0,  1,  1,  1)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelTwo #
  EThreR2 (Lambda_E)=  0.500D-06(au)
****************************
        SINGLET STATE
****************************
------------------------------------------------------------
LINKED OPERATORS FOR SAC:    SYMMETRY = AG  GROUND STATE
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            63        9024         9087
    AFTER             63        3492         3556
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AG  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.296334
       8 ->  17     0.94023        8 ->  25     0.32851
    ##   2-nd state ##       energy (au) =       0.380223
       8 ->  25     0.92052        8 ->  17    -0.33907
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            63        9024         9087
    AFTER             63        1980         2044
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.281843
```

Compared with the "LevelOne" threshold in the former input, the number of selected operators increased The same is for all the states.

```
      8 ->  11     0.86335        8 ->  23     0.48630
      8 ->  29     0.10227
   ##   2-nd state ##       energy (au) =       0.341571
      7 ->  18     0.72120        7 ->  27    -0.64239
      7 ->  14     0.14162        8 ->  23     0.11167
      7 ->  36    -0.11143        8 ->  11    -0.11010
   ##   3-th state ##       energy (au) =       0.356963
      8 ->  23     0.82116        8 ->  11    -0.49204
      8 ->  29     0.19651        8 ->  34    -0.12686
      7 ->  18    -0.12591        7 ->  27     0.10502
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            29        7364         7393
    AFTER             29        3298         3327
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2G EXCITED STATE
  #SECI# Main reference configuration and coefficient
   ##   1-st state ##       energy (au) =       0.287373
      8 ->  10     0.91243        8 ->  24     0.39911
   ##   2-nd state ##       energy (au) =       0.369257
      8 ->  24     0.81584        8 ->  10    -0.38382
      6 ->  27    -0.27427        6 ->  18     0.26566
      8 ->  31    -0.17400
   ##   3-th state ##       energy (au) =       0.376304
      6 ->  27     0.63715        6 ->  18    -0.62072
      8 ->  24     0.37166        6 ->  36     0.15588
      8 ->  10    -0.14036        6 ->  14    -0.10387
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            35        7484         7519
    AFTER             35        3309         3344
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE
  #SECI# Main reference configuration and coefficient
   ##   1-st state ##       energy (au) =       0.386987
      7 ->   9     0.87379        7 ->  26     0.37236
      7 ->  19    -0.16572        7 ->  16     0.14314
      5 ->  24     0.11788
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            53        8708         8761
    AFTER             53        2492         2545
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AU  EXCITED STATE
  #SECI# Main reference configuration and coefficient
   ##   1-st state ##       energy (au) =       0.320962
      8 ->  12     0.90268        8 ->  22     0.42641
   ##   2-nd state ##       energy (au) =       0.368854
      8 ->  22     0.89326        8 ->  12    -0.43030
      8 ->  33     0.12187
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            27        7356         7383
```

```
    AFTER              27        1422         1449
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.284181
       8 ->  18     0.82474        8 ->  27    -0.40146
       8 ->  14     0.33925
    ##   2-nd state ##       energy (au) =       0.331060
       8 ->  14     0.91523        8 ->  27     0.34202
       8 ->  18    -0.18352
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            61        8836         8897
    AFTER             61        2408         2469
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.320792
       8 ->  15     0.88807        8 ->  20     0.45915
    ##   2-nd state ##       energy (au) =       0.364234
       8 ->  20     0.88703        8 ->  15    -0.45967
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            55        8716         8771
    AFTER             55         821          876
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.260350
       8 ->   9     0.89702        8 ->  26     0.35048
       8 ->  16     0.17828        8 ->  19    -0.16415
    ##   2-nd state ##       energy (au) =       0.315645
       8 ->  13     0.72791        8 ->  19     0.57881
       8 ->  16     0.34382        8 ->  28     0.11322
    ##   3-th state ##       energy (au) =       0.319844
       8 ->  16     0.77242        8 ->  21    -0.48071
       8 ->  13    -0.38277        8 ->   9    -0.14211
    ##   4-th state ##       energy (au) =       0.348811
       8 ->  19     0.65807        8 ->  13    -0.49993
       8 ->   9     0.34671        8 ->  26    -0.34490
       8 ->  28     0.20148        8 ->  16    -0.17875
    ##   5-th state ##       energy (au) =       0.361679
       8 ->  21     0.82835        8 ->  16     0.46809
       8 ->  26    -0.20355        8 ->  19    -0.13967
       8 ->  13    -0.13875
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            37        7492         7529
    AFTER             37        2569         2606
****************************
        TRIPLET STATE
****************************
```

```
-----------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AG  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.284276
       8 ->  17     0.86842        8 ->  25     0.48460
    ##   2-nd state ##       energy (au) =       0.363288
       8 ->  25     0.85196        8 ->  17    -0.49556
       8 ->  35    -0.15070
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            63       12189        12252
    AFTER             63        1573         1636
-----------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.278966
       8 ->  11     0.83989        8 ->  23     0.51633
       8 ->  29     0.12821
    ##   2-nd state ##       energy (au) =       0.316463
       7 ->  18     0.70581        7 ->  27    -0.67742
       7 ->  14     0.12567        7 ->  36    -0.12532
    ##   3-th state ##       energy (au) =       0.352620
       8 ->  23     0.79138        8 ->  11    -0.53814
       8 ->  29     0.24969        8 ->  34    -0.13223
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            29       10500        10529
    AFTER             29        4188         4217
-----------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.283348
       8 ->  10     0.88446        8 ->  24     0.44379
       8 ->  31    -0.13053
    ##   2-nd state ##       energy (au) =       0.347308
       6 ->  27     0.69974        6 ->  18    -0.64978
       6 ->  36     0.18078        8 ->  10     0.10859
       8 ->  24    -0.10797        6 ->  14    -0.10124
    ##   3-th state ##       energy (au) =       0.364354
       8 ->  24     0.84635        8 ->  10    -0.45313
       8 ->  31    -0.21638        6 ->  27     0.11741
       6 ->  18    -0.10643
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            35       10602        10637
    AFTER             35        4222         4257
-----------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.370044
       7 ->   9     0.77647        7 ->  26     0.44073
       7 ->  19    -0.21913        7 ->  28    -0.17447
```

```
      5 ->  24     0.17377        5 ->  10     0.11183
      7 ->  16     0.11173
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            53       12222        12275
    AFTER             53        3626         3679
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AU  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.320525
      8 ->  12     0.89588        8 ->  22     0.43915
    ##   2-nd state ##       energy (au) =       0.367583
      8 ->  22     0.88376        8 ->  12    -0.44423
      8 ->  33     0.13093
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            27       10506        10533
    AFTER             27        1698         1725
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.129560
      8 ->  27     0.71782        8 ->  18    -0.66032
      8 ->  36     0.17938        8 ->  14    -0.10220
    ##   2-nd state ##       energy (au) =       0.324207
      8 ->  14     0.93866        8 ->  27     0.28541
      8 ->  18     0.18242
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            61       12318        12379
    AFTER             61        2128         2189
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.319743
      8 ->  15     0.86916        8 ->  20     0.49394
    ##   2-nd state ##       energy (au) =       0.361471
      8 ->  20     0.86729        8 ->  15    -0.49439
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            55       12240        12295
    AFTER             55         995         1050
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.252381
      8 ->   9     0.85547        8 ->  26     0.42815
      8 ->  16     0.19023        8 ->  19    -0.16184
    ##   2-nd state ##       energy (au) =       0.313559
      8 ->  16     0.62658        8 ->  19     0.54898
      8 ->  13     0.40646        8 ->  21    -0.32387
      8 ->  28     0.15678
    ##   3-th state ##       energy (au) =       0.315979
```

```
      8 ->  13     0.68320        8 ->  21     0.49464
      8 ->  16    -0.38839        8 ->  19     0.26803
      8 ->   9     0.20236        8 ->  26    -0.11168
      8 ->  32     0.10498
   ##   4-th state ##       energy (au) =       0.345015
      8 ->  13     0.53277        8 ->  19    -0.50357
      8 ->  26     0.47087        8 ->   9    -0.39931
      8 ->  21    -0.20178        8 ->  28    -0.17378
   ##   5-th state ##       energy (au) =       0.350851
      8 ->  16     0.64554        8 ->  21     0.60356
      8 ->  19    -0.35868        8 ->  26    -0.20475
      8 ->  28    -0.16720        8 ->  32     0.11453
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            37       10593        10630
    AFTER             37        3158         3195
****************************
       IONIZED STATE
****************************
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AG  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.585304
      6     1.00000
    ##   2-nd state ##       energy (au) =       1.033118
      3     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             2         332          334
    AFTER              2         320          322
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.508192
      7     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1         312          313
    AFTER              1         269          270
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.792389
      4     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1         328          329
    AFTER              1         282          283
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.643034
      5     1.00000
```

```
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1         316         317
    AFTER              1         276         277
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.374824
       8     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1         228         229
    AFTER              1         196         197
=================================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
=================================================================
=================================================================
  STEP #DIAGCI#  Solution of SDCI
=================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   AG    CONVERGED
Solution for Singlet   AG    CONVERGED
Solution for Singlet   B1G   CONVERGED
Solution for Singlet   B2G   CONVERGED
Solution for Singlet   B3G   CONVERGED
Solution for Singlet   AU    CONVERGED
Solution for Singlet   B1U   CONVERGED
Solution for Singlet   B2U   CONVERGED
Solution for Singlet   B3U   CONVERGED
=================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
=================================================================
Threshold for S2 operator (CThreULS2G) 0.500D-02
=================================================================
  STEP #SAC#  Solution of SAC equation
=================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-05
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Solution for SAC equation converged
*****************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*****************************************
HF ENERGY     =     -78.050872 (AU)
SAC-NV  ENERGY=      -0.271572 (AU)
TOTAL ENERGY  =     -78.322445 (AU)
SAC-NV  coefficients (|C|>=0.03)
*SINGLE EXCITATION
```

```
*DOUBLE EXCITATION
       8   27    8   18      0.11618         8   27    8   27     -0.08411
       8   36    8   27     -0.07699         8   36    8   18      0.04960
       8   27    6   38     -0.04796         8   18    8   18     -0.04091
       8   36    6   38     -0.03942         8   27    3   31      0.03180
       8   18    6   38      0.03023
Hartree-Fock configuration   1.00000
=====================================================================
  STEP #ULINTS#  Unlinked integral for Singlet Excited State (SAC-CI)
=====================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
=============================================================
  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
=============================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   AG    CONVERGED
Solution for Singlet   B1G   CONVERGED
Solution for Singlet   B2G   CONVERGED
Solution for Singlet   B3G   CONVERGED
Solution for Singlet   AU    CONVERGED
Solution for Singlet   B1U   CONVERGED
Solution for Singlet   B2U   CONVERGED
Solution for Singlet   B3U   CONVERGED
***********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
***********************************************
*****************************************************************************
Singlet       AG      ******************************************************
###   1-st  ###           ---   5th state in this spin multiplicity ---
    Total energy       in au =     -78.021504
    Correlation energy in au =       0.029368
    Excitation energy  in au =       0.300940    in eV =       8.189000
  *SINGLE EXCITATION
       8   17     0.91523         8   25     0.32686
  *DOUBLE EXCITATION
       8   25    8   17    -0.10493         8   35    8   17     0.08707
       8   17    7   33    -0.07094         8   17    5   29    -0.06421
       8   17    6   32    -0.06215         8   17    4   31     0.06002
       8   17    5   23    -0.05578         8   17    5   34     0.05237
       8   17    7   37     0.04854         8   36    8   27     0.04340
       8   27    8   27     0.03908         8   17    4   24    -0.03422
       8   17    7   22    -0.03371         8   25    8   25    -0.03257
       8   17    8   17    -0.03014
###   2-nd  ###           ---  20th state in this spin multiplicity ---
    Total energy       in au =     -77.936302
    Correlation energy in au =       0.114570
    Excitation energy  in au =       0.386143    in eV =      10.507482
```

```
  *SINGLE EXCITATION
       8   25     0.89991         8   17    -0.33633
       8   35    -0.09029         7   22    -0.07011
       6    9    -0.05451         7   33    -0.03061
  *DOUBLE EXCITATION
       8   25    8   25    -0.09049         8   35    8   25     0.08922
       8   36    8   27     0.07417         8   25    7   33    -0.06208
       8   27    8   27     0.05676         8   25    5   29    -0.05401
       8   25    6   32    -0.05382         8   27    8   18    -0.05305
       8   25    4   31     0.05252         8   36    8   18    -0.04619
       8   25    5   34     0.03909         8   25    5   23    -0.03857
       8   25    7   37     0.03450         8   35    8   17    -0.03111
*****************************************************************************
Singlet       B1G     ******************************************************
###   1-st  ###           ---   2nd state in this spin multiplicity ---
    Total energy       in au =     -78.034408
    Correlation energy in au =       0.016464
    Excitation energy  in au =       0.288036    in eV =       7.837865
  *SINGLE EXCITATION
       8   11     0.85237         8   23     0.45929
       8   29     0.08655         8   34    -0.07000
       7   18     0.04107         7   27    -0.03853
  *DOUBLE EXCITATION
       8   25    8   11    -0.08352         8   35    8   11     0.07807
       8   11    7   33    -0.06585         8   11    5   29    -0.06030
       8   11    6   32    -0.05792         8   11    4   31     0.05678
       8   11    5   23    -0.05268         8   11    5   34     0.04153
       8   25    8   23    -0.04044         8   11    7   37     0.03883
       8   35    8   23     0.03592         8   11    4   24    -0.03200
       8   11    7   22    -0.03192         8   33    8   27     0.03080
###   2-nd  ###           ---   9th state in this spin multiplicity ---
    Total energy       in au =     -77.996322
    Correlation energy in au =       0.054550
    Excitation energy  in au =       0.326122    in eV =       8.874244
  *SINGLE EXCITATION
       7   18     0.71585         7   27    -0.61527
       7   14     0.14319         7   36    -0.11233
       8   11    -0.08924         8   29     0.05745
  *DOUBLE EXCITATION
       8   27    5   18    -0.11836         8   27    5   27     0.11018
       8   18    5   18     0.09214         8   18    5   27    -0.09129
       8   36    5   18    -0.03986         7   30    4   27     0.03575
       7   30    4   18    -0.03569         8   35    7   36     0.03428
       7   29    5   18     0.03292         7   43    4   27    -0.03237
       7   43    4   18     0.03199         6   38    5   18    -0.03198
       7   29    5   27    -0.03169         8   36    5   27     0.03042
###   3-rd  ###           ---  14th state in this spin multiplicity ---
    Total energy       in au =     -77.956826
    Correlation energy in au =       0.094046
```

```
   Excitation energy  in au =       0.365618    in eV =       9.948982
  *SINGLE EXCITATION
      8   23     0.82630         8   11    -0.46666
      8   29     0.18045         8   34    -0.12421
      7   18    -0.06552         7   27     0.04430
  *DOUBLE EXCITATION
      8   25    8   23    -0.07475         8   35    8   23     0.06858
      8   23    7   33    -0.05571         8   23    5   29    -0.05297
      8   25    8   11     0.04984         8   35    8   11    -0.04742
      8   33    8   27     0.04412         8   23    4   31     0.04322
      8   23    5   23    -0.04104         8   23    6   32    -0.04034
      8   11    7   33     0.04011         8   23    5   34     0.03672
      8   11    5   29     0.03608         8   11    6   32     0.03605
      8   11    4   31    -0.03375         8   23    7   37     0.03324
      8   11    5   23     0.03132
*****************************************************************************
Singlet       B2G     ******************************************************
###   1-st  ###           ---   3rd state in this spin multiplicity ---
   Total energy       in au =     -78.033630
   Correlation energy in au =       0.017242
   Excitation energy  in au =       0.288815    in eV =       7.859047
  *SINGLE EXCITATION
      8   10     0.87445         8   24     0.41622
      8   31    -0.09160
  *DOUBLE EXCITATION
      8   25    8   10    -0.08524         8   35    8   10     0.07972
      8   10    7   33    -0.06774         8   10    5   29    -0.06698
      8   10    6   32    -0.06301         8   10    4   31     0.06150
      8   10    5   23    -0.05292         8   10    7   37     0.04957
      8   10    5   34     0.04106         8   27    8    9     0.04089
      8   26    8   18    -0.04047         8   27    8   26     0.03984
      8   25    8   24    -0.03706         8   10    4   24    -0.03473
      8   10    7   22    -0.03332         8   35    8   24     0.03316
      8   24    5   29    -0.03287
###   2-nd  ###           ---  17th state in this spin multiplicity ---
   Total energy       in au =     -77.951908
   Correlation energy in au =       0.098964
   Excitation energy  in au =       0.370537    in eV =      10.082815
  *SINGLE EXCITATION
      8   24     0.72560         8   10    -0.38558
      6   18     0.34880         6   27    -0.32354
      8   31    -0.17733         6   36    -0.07176
      6   14     0.06179         8   30    -0.05297
  *DOUBLE EXCITATION
      8   25    8   24    -0.06670         8   27    8   26     0.06397
      8   35    8   24     0.06144         8   26    8   18    -0.05499
      8   24    5   29    -0.05459         8   24    7   33    -0.05097
      8   24    6   32    -0.05062         8   24    4   31     0.05023
      8   27    4   27     0.04952         8   27    4   18    -0.04766
```

```
      8   25    8   10     0.04129         8   35    8   10    -0.03931
      8   10    7   33     0.03290         8   24    5   23    -0.03279
      8   24    7   37     0.03276         8   18    4   27    -0.03193
      8   24    4   24    -0.03080         8   24    5   34     0.03074
      8   32    8   27     0.03052         8   27    8    9     0.03045
      8   18    4   18     0.03041
###   3-rd  ###          ---  19th state in this spin multiplicity ---
    Total energy       in au =     -77.944766
    Correlation energy in au =       0.106106
    Excitation energy  in au =       0.377679    in eV =      10.277166
  *SINGLE EXCITATION
      6   18    -0.60566         6   27     0.55774
      8   24     0.44887         8   10    -0.19262
      6   36     0.12388         6   14    -0.11349
      3   27    -0.05201         8   31    -0.04460
      3   18     0.03286
  *DOUBLE EXCITATION
      8   27    4   18     0.06312         8   27    4   27    -0.05422
      8   18    4   18    -0.05337         8   18    4   27     0.04983
      8   25    8   24    -0.04286         8   35    8   24     0.03956
      8   24    5   29    -0.03409         8   27    8   26     0.03256
      8   24    7   33    -0.03227         6   38    4   18     0.03182
      6   38    4   27    -0.03109         8   24    4   31     0.03059
*****************************************************************************
Singlet       B3G     ******************************************************
###   1-st  ###          ---  13th state in this spin multiplicity ---
    Total energy       in au =     -77.962758
    Correlation energy in au =       0.088114
    Excitation energy  in au =       0.359687    in eV =       9.787571
  *SINGLE EXCITATION
      7    9     0.87422         7   26     0.34063
      7   19    -0.16158         7   16     0.13303
      7   28    -0.06940         7   13     0.06410
  *DOUBLE EXCITATION
      8   27    5    9    -0.12118         8   18    5    9     0.08309
      8   35    7    9     0.06826         8   25    7    9    -0.06721
      8   36    5    9    -0.06007         7   33    7    9    -0.05089
      8   27    5   26    -0.04269         6   38    5    9    -0.03796
      7   29    5    9     0.03568         6   29    4    9     0.03298
      7    9    5   23    -0.03233         7   30    4    9    -0.03187
      7    9    5   34     0.03099         7   43    4    9     0.03003
*****************************************************************************
Singlet       AU      ******************************************************
###   1-st  ###          ---   7th state in this spin multiplicity ---
    Total energy       in au =     -77.997096
    Correlation energy in au =       0.053776
    Excitation energy  in au =       0.325348    in eV =       8.853173
  *SINGLE EXCITATION
      8   12     0.87668         8   22     0.42389
```

```
      8   33     0.04918
  *DOUBLE EXCITATION
      8   25    8   12    -0.08738         8   35    8   12     0.08211
      8   12    7   33    -0.07021         8   12    5   29    -0.06513
      8   12    6   32    -0.06235         8   12    4   31     0.06033
      8   12    5   23    -0.05570         8   12    5   34     0.05131
      8   12    7   37     0.04970         8   25    8   22    -0.03995
      8   35    8   22     0.03697         8   12    7   22    -0.03473
      8   12    4   24    -0.03396         8   22    7   33    -0.03264
      8   22    5   29    -0.03211
###   2-nd  ###           ---  18th state in this spin multiplicity ---
    Total energy       in au =     -77.948813
    Correlation energy in au =       0.102059
    Excitation energy  in au =       0.373632    in eV =      10.167043
  *SINGLE EXCITATION
      8   22     0.86867         8   12    -0.42748
      8   33     0.11119
  *DOUBLE EXCITATION
      8   25    8   22    -0.08311         8   35    8   22     0.07724
      8   22    7   33    -0.06697         8   22    5   29    -0.06490
      8   22    6   32    -0.06038         8   22    4   31     0.05941
      8   22    5   23    -0.05240         8   22    7   37     0.04865
      8   25    8   12     0.04377         8   35    8   12    -0.04131
      8   27    8   23     0.04073         8   22    5   34     0.04054
      8   22    7   22    -0.03604         8   12    7   33     0.03473
      8   22    4   24    -0.03259         8   12    5   29     0.03140
      8   12    6   32     0.03064
*****************************************************************************
Singlet       B1U     ******************************************************
###   1-st  ###           ---   4th state in this spin multiplicity ---
    Total energy       in au =     -78.022947
    Correlation energy in au =       0.027925
    Excitation energy  in au =       0.299498    in eV =       8.149742
  *SINGLE EXCITATION
      8   18     0.80653         8   14     0.42089
      8   27    -0.34020         6   38     0.06738
      7   29    -0.06169         7   23     0.04661
      4   26     0.04536         6   30    -0.03981
      5   33     0.03318         7   34    -0.03236
  *DOUBLE EXCITATION
      8   36    8   35     0.05403         8   18    5   29    -0.05147
      8   25    8   18    -0.04199         8   25    8   14    -0.03929
      8   35    8   18     0.03879         8   35    8   14     0.03693
      8   18    7   33    -0.03288         8   18    6   32    -0.03216
      8   18    4   31     0.03193         8   14    7   33    -0.03071
      8   14    5   29    -0.03030         8   36    8   25    -0.03000
###   2-nd  ###           ---  11th state in this spin multiplicity ---
    Total energy       in au =     -77.983975
    Correlation energy in au =       0.066897
```

```
    Excitation energy  in au =       0.338470    in eV =       9.210230
  *SINGLE EXCITATION
       8   14     0.85962         8   27     0.34862
       8   18    -0.29342         6   38    -0.03878
       7   23    -0.03829         7   29     0.03150
  *DOUBLE EXCITATION
       8   25    8   14    -0.08967         8   35    8   14     0.08392
       8   14    7   33    -0.07028         8   14    5   29    -0.06388
       8   14    6   32    -0.06226         8   14    4   31     0.05999
       8   14    5   23    -0.05588         8   14    5   34     0.05149
       8   14    7   37     0.04936         8   14    7   22    -0.03459
       8   14    4   24    -0.03418         8   36    8   35    -0.03207
       8   17    8   14    -0.03062
*****************************************************************************
Singlet       B2U     ******************************************************
###   1-st  ###           ---  10th state in this spin multiplicity ---
    Total energy       in au =     -77.996062
    Correlation energy in au =       0.054810
    Excitation energy  in au =       0.326382    in eV =       8.881310
  *SINGLE EXCITATION
       8   15     0.87099         8   20     0.43956
  *DOUBLE EXCITATION
       8   25    8   15    -0.08838         8   35    8   15     0.08297
       8   15    7   33    -0.06974         8   15    5   29    -0.06315
       8   15    6   32    -0.06121         8   15    4   31     0.05898
       8   15    5   23    -0.05534         8   15    5   34     0.05150
       8   15    7   37     0.04825         8   25    8   20    -0.04761
       8   35    8   20     0.04317         8   20    7   33    -0.03444
       8   15    7   22    -0.03394         8   15    4   24    -0.03351
###   2-nd  ###           ---  16th state in this spin multiplicity ---
    Total energy       in au =     -77.952020
    Correlation energy in au =       0.098852
    Excitation energy  in au =       0.370425    in eV =      10.079775
  *SINGLE EXCITATION
       8   20     0.87117         8   15    -0.43947
  *DOUBLE EXCITATION
       8   25    8   20    -0.09384         8   35    8   20     0.08532
       8   20    7   33    -0.06825         8   20    5   29    -0.05956
       8   20    6   32    -0.05904         8   20    4   31     0.05683
       8   20    5   23    -0.05407         8   20    5   34     0.05190
       8   25    8   15     0.04353         8   35    8   15    -0.04149
       8   20    7   37     0.03862         8   15    7   33     0.03532
       8   15    5   29     0.03273         8   20    4   24    -0.03248
       8   20    7   22    -0.03209         8   15    6   32     0.03144
       8   15    4   31    -0.03028
*****************************************************************************
Singlet       B3U     ******************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    Total energy       in au =     -78.058092
```

```
    Correlation energy in au =      -0.007220
    Excitation energy  in au =       0.264353    in eV =       7.193408
  *SINGLE EXCITATION
       8    9     0.87859         8   26     0.34016
       8   16     0.16640         8   19    -0.15048
       8   13     0.07498         8   28    -0.07382
       8   32     0.03999
  *DOUBLE EXCITATION
       8   25    8    9    -0.08920         8   35    8    9     0.08152
       8    9    7   33    -0.06598         8    9    5   29    -0.06246
       8    9    6   32    -0.05927         8    9    4   31     0.05807
       8    9    5   23    -0.05235         8   27    8   24     0.04557
       8    9    5   34     0.04183         8    9    7   37     0.03943
       8   26    8   25    -0.03422         8    9    4   24    -0.03177
       8    9    7   22    -0.03156         8   24    8   18    -0.03112
###   2-nd  ###           ---   6th state in this spin multiplicity ---
    Total energy       in au =     -77.999995
    Correlation energy in au =       0.050877
    Excitation energy  in au =       0.322450    in eV =       8.774309
  *SINGLE EXCITATION
       8   13     0.75116         8   19     0.54783
       8   16     0.26877         8   28     0.10830
       8   21     0.06343         8   26    -0.03665
       8   32     0.03338
  *DOUBLE EXCITATION
       8   25    8   13    -0.07535         8   35    8   13     0.07096
       8   13    7   33    -0.05903         8   13    5   29    -0.05541
       8   13    6   32    -0.05408         8   25    8   19    -0.05338
       8   13    4   31     0.05199         8   35    8   19     0.05055
       8   13    5   23    -0.03804         8   13    5   34     0.03601
       8   13    7   37     0.03583         8   19    7   33    -0.03492
       8   19    5   29    -0.03198         8   19    4   31     0.03188
       8   19    6   32    -0.03127
###   3-rd  ###           ---   8th state in this spin multiplicity ---
    Total energy       in au =     -77.996334
    Correlation energy in au =       0.054538
    Excitation energy  in au =       0.326111    in eV =       8.873923
  *SINGLE EXCITATION
       8   16    -0.78400         8   21     0.47226
       8   13     0.30211         8    9     0.11743
       8   19    -0.08239         8   32     0.04347
       8   28    -0.03045
  *DOUBLE EXCITATION
       8   25    8   16     0.08189         8   35    8   16    -0.07630
       8   16    7   33     0.06150         8   16    5   29     0.05598
       8   16    6   32     0.05500         8   25    8   21    -0.05390
       8   16    4   31    -0.05251         8   16    5   23     0.04848
       8   35    8   21     0.04780         8   16    5   34    -0.03833
       8   16    7   37    -0.03602         8   21    7   33    -0.03500
```

```
      8   21    5   29    -0.03275         8   21    6   32    -0.03215
      8   21    4   31     0.03074         8   16    4   24     0.03007
      8   16    7   22     0.03002
###   4-th  ###          ---  12th state in this spin multiplicity ---
    Total energy       in au =     -77.965479
    Correlation energy in au =       0.085393
    Excitation energy  in au =       0.356965    in eV =       9.713512
  *SINGLE EXCITATION
      8   19     0.66863         8   13    -0.46343
      8    9     0.33089         8   26    -0.31979
      8   28     0.20955         8   16    -0.19489
  *DOUBLE EXCITATION
      8   25    8   19    -0.06404         8   35    8   19     0.06102
      8   25    8   13     0.04691         8   35    8   13    -0.04414
      8   19    7   33    -0.04186         8   19    5   29    -0.03779
      8   19    4   31     0.03777         8   19    6   32    -0.03685
      8   13    7   33     0.03678         8   25    8    9    -0.03594
      8   13    5   29     0.03352         8   19    5   34     0.03321
      8   13    6   32     0.03280         8   35    8    9     0.03267
      8   19    5   23    -0.03243         8   13    4   31    -0.03143
###   5-th  ###          ---  15th state in this spin multiplicity ---
    Total energy       in au =     -77.954115
    Correlation energy in au =       0.096757
    Excitation energy  in au =       0.368330    in eV =      10.022756
  *SINGLE EXCITATION
      8   21    -0.82441         8   16    -0.44240
      8   13     0.18560         8   26     0.16268
      8   32    -0.09340         8   19     0.06445
      8   28     0.05108
  *DOUBLE EXCITATION
      8   25    8   21     0.09429         8   35    8   21    -0.08448
      8   21    7   33     0.06154         8   21    5   29     0.05709
      8   21    6   32     0.05624         8   21    4   31    -0.05385
      8   21    5   23     0.04822         8   25    8   16     0.04149
      8   35    8   16    -0.04055         8   21    5   34    -0.03855
      8   21    7   37    -0.03638         8   16    7   33     0.03550
      8   16    5   29     0.03338         8   16    6   32     0.03214
      8   16    4   31    -0.03093         8   21    4   24     0.03025
================================================================
  STEP #DENS#  Density Calculation
================================================================
Transition density for SAC/SAC-CI (V)
Threshold for S2 operators (CThreDensULS2):  0.50D-02
Threshold for R1,R2 operators (CThreDensULR1):  0.10D+00
Only right vectors are used. (ILEFT=0)
--------------------------------------------------------------------------------
Transition dipole moment of   singlet state from SAC ground state
--------------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
```

```
                    energy (eV)       X           Y           Z       strength
-------------------------------------------------------------------------------
   AG         0       0.0          Excitations are from this state.
   AG         1       8.1890      0.0000      0.0000      0.0000      0.0000
   AG         2      10.5075      0.0000      0.0000      0.0000      0.0000
   B1G        1       7.8379      0.0000      0.0000      0.0000      0.0000
   B1G        2       8.8742      0.0000      0.0000      0.0000      0.0000
   B1G        3       9.9490      0.0000      0.0000      0.0000      0.0000
   B2G        1       7.8590      0.0000      0.0000      0.0000      0.0000
   B2G        2      10.0828      0.0000      0.0000      0.0000      0.0000
   B2G        3      10.2772      0.0000      0.0000      0.0000      0.0000
   B3G        1       9.7876      0.0000      0.0000      0.0000      0.0000
   AU         1       8.8532      0.0000      0.0000      0.0000      0.0000
   AU         2      10.1670      0.0000      0.0000      0.0000      0.0000
   B1U        1       8.1497      0.0000      0.0000     -1.3487      0.3632
   B1U        2       9.2102      0.0000      0.0000      0.5263      0.0625
   B2U        1       8.8813      0.0000     -0.3093      0.0000      0.0208
   B2U        2      10.0798      0.0000     -0.4255      0.0000      0.0447
   B3U        1       7.1934     -0.6744      0.0000      0.0000      0.0802
   B3U        2       8.7743     -0.1444      0.0000      0.0000      0.0045
   B3U        3       8.8739      0.4793      0.0000      0.0000      0.0499
   B3U        4       9.7135      0.0335      0.0000      0.0000      0.0003
   B3U        5      10.0228     -0.6751      0.0000      0.0000      0.1119
-------------------------------------------------------------------------------
================================================================
  STEP #CIMX#  CI matrix elements          ### TRIPLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Triplet   AG    CONVERGED
Solution for Triplet   B1G   CONVERGED
Solution for Triplet   B2G   CONVERGED
Solution for Triplet   B3G   CONVERGED
Solution for Triplet   AU    CONVERGED
Solution for Triplet   B1U   CONVERGED
Solution for Triplet   B2U   CONVERGED
Solution for Triplet   B3U   CONVERGED
================================================================
  STEP #ULINTT#  Unlinked integral for Triplet State (SAC-CI)
================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
================================================================
  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
================================================================
Threshold for density convergence (DConvDiag) .100D-03
```

```
Maximum number of iteration (MaxItDiag)    64
Solution for Triplet   AG    CONVERGED
Solution for Triplet   B1G   CONVERGED
Solution for Triplet   B2G   CONVERGED
Solution for Triplet   B3G   CONVERGED
Solution for Triplet   AU    CONVERGED
Solution for Triplet   B1U   CONVERGED
Solution for Triplet   B2U   CONVERGED
Solution for Triplet   B3U   CONVERGED
**********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
**********************************************
*******************************************************************************
Triplet       AG      ***********************************************************
###   1-st  ###           ---   5th state in this spin multiplicity ---
    Total energy       in au =     -78.027163
    Correlation energy in au =       0.023709
    Excitation energy  in au =       0.295281    in eV =       8.035011
  *SINGLE EXCITATION
       8   17     0.88461         8   25     0.41082
       8   35    -0.06881
  *DOUBLE EXCITATION
       8   35    8   17     0.08416         8   25    8   17    -0.07456
       7   33    8   17    -0.06974         5   29    8   17    -0.06339
       6   32    8   17    -0.06041         4   31    8   17     0.05913
       5   23    8   17    -0.05435         5   34    8   17     0.05050
       7   37    8   17     0.04772         8   35    8   25     0.03793
       4   24    8   17    -0.03306         7   22    8   17    -0.03251
###   2-nd  ###           ---  20th state in this spin multiplicity ---
    Total energy       in au =     -77.945600
    Correlation energy in au =       0.105272
    Excitation energy  in au =       0.376845    in eV =      10.254464
  *SINGLE EXCITATION
       8   25     0.87749         8   17    -0.41214
       8   35    -0.13665
  *DOUBLE EXCITATION
       8   35    8   25     0.07829         8   25    8   17     0.07764
       7   33    8   25    -0.06104         6   32    8   25    -0.05612
       5   29    8   25    -0.05560         4   31    8   25     0.05364
       8   35    8   17    -0.04234         5   34    8   25     0.03844
       5   25    8   23     0.03759         8   25    5   23     0.03698
       7   33    8   17     0.03618         7   37    8   25     0.03441
       8   23    5   25     0.03347         5   29    8   17     0.03311
       6   32    8   17     0.03126         4   31    8   17    -0.03030
*******************************************************************************
Triplet       B1G     ***********************************************************
###   1-st  ###           ---   4th state in this spin multiplicity ---
    Total energy       in au =     -78.035527
    Correlation energy in au =       0.015345
```

```
    Excitation energy  in au =       0.286917    in eV =       7.807409
  *SINGLE EXCITATION
       8   11     0.84423         8   23     0.47228
       8   29     0.09748         8   34    -0.07744
       7   27     0.04227         7   18    -0.03752
  *DOUBLE EXCITATION
       8   25    8   11    -0.08173         8   35    8   11     0.07755
       7   33    8   11    -0.06682         5   29    8   11    -0.06066
       6   32    8   11    -0.05728         4   31    8   11     0.05720
       5   23    8   11    -0.04453         5   34    8   11     0.04210
       7   37    8   11     0.03940         8   25    8   23    -0.03893
       8   35    8   23     0.03787         7   33    8   23    -0.03188
       4   24    8   11    -0.03134         7   22    8   11    -0.03029
###   2-nd  ###           ---   6th state in this spin multiplicity ---
    Total energy       in au =     -78.008171
    Correlation energy in au =       0.042701
    Excitation energy  in au =       0.314274    in eV =       8.551826
  *SINGLE EXCITATION
       7   18     0.70891         7   27    -0.63762
       7   14     0.13423         7   36    -0.11938
       8   11     0.07129
  *DOUBLE EXCITATION
       8   27    5   18    -0.10704         8   27    5   27     0.08990
       8   18    5   27    -0.07355         8   18    5   18     0.07246
       8   36    5   18    -0.03789         8   35    7   36     0.03579
       6   38    5   18    -0.03278
###   3-rd  ###           ---  16th state in this spin multiplicity ---
    Total energy       in au =     -77.958773
    Correlation energy in au =       0.092099
    Excitation energy  in au =       0.363672    in eV =       9.896017
  *SINGLE EXCITATION
       8   23     0.81340         8   11    -0.48417
       8   29     0.20549         8   34    -0.12884
       7   18     0.03939
  *DOUBLE EXCITATION
       8   25    8   23    -0.07128         8   35    8   23     0.06813
       7   33    8   23    -0.05627         8   25    8   11     0.05228
       8   35    8   11    -0.04875         5   23    8   11     0.04845
       4   31    8   23     0.04233         7   33    8   11     0.04162
       5   29    8   23    -0.04068         5   29    8   11     0.03930
       6   32    8   23    -0.03890         5   34    8   23     0.03769
       6   32    8   11     0.03747         4   31    8   11    -0.03529
       7   37    8   23     0.03470         8   33    8   27    -0.03220
       8   23    5   23     0.03108
*****************************************************************************
Triplet       B2G     ******************************************************
###   1-st  ###           ---   3rd state in this spin multiplicity ---
    Total energy       in au =     -78.035822
    Correlation energy in au =       0.015050
```

```
    Excitation energy  in au =       0.286623    in eV =       7.799396
  *SINGLE EXCITATION
       8   10     0.86087         8   24     0.43880
       8   31    -0.12071
  *DOUBLE EXCITATION
       8   25    8   10    -0.08313         8   35    8   10     0.07890
       7   33    8   10    -0.06758         5   29    8   10    -0.06671
       6   32    8   10    -0.06211         4   31    8   10     0.06040
       5   23    8   10    -0.05244         7   37    8   10     0.04960
       5   34    8   10     0.04055         8   27    8   26     0.04018
       8   27    8    9     0.04003         8   25    8   24    -0.03679
       8   35    8   24     0.03607         5   29    8   24    -0.03324
       7   22    8   10    -0.03106
###   2-nd  ###           ---  13th state in this spin multiplicity ---
    Total energy       in au =     -77.967316
    Correlation energy in au =       0.083556
    Excitation energy  in au =       0.355128    in eV =       9.663527
  *SINGLE EXCITATION
       6   18    -0.67899         6   27     0.66738
       6   36     0.15889         6   14    -0.11637
       8   24    -0.04744         3   27    -0.04491
       8   10     0.04338
  *DOUBLE EXCITATION
       8   27    4   18     0.07507         8   27    4   27    -0.06797
       8   18    4   27     0.05442         8   18    4   18    -0.05231
       8   35    6   18    -0.03346         8   36    6   35    -0.03272
       8   35    6   36    -0.03231
###   3-rd  ###           ---  18th state in this spin multiplicity ---
    Total energy       in au =     -77.953253
    Correlation energy in au =       0.097619
    Excitation energy  in au =       0.369192    in eV =      10.046211
  *SINGLE EXCITATION
       8   24     0.82989         8   10    -0.45556
       8   31    -0.21403         6   27     0.04699
       8   40     0.04666         6   18    -0.04206
       8   30    -0.03876
  *DOUBLE EXCITATION
       8   25    8   24    -0.07444         8   35    8   24     0.07193
       5   29    8   24    -0.06086         8   27    8   26     0.05596
       7   33    8   24    -0.05569         6   32    8   24    -0.05464
       4   31    8   24     0.05294         8   25    8   10     0.04906
       8   35    8   10    -0.04540         7   33    8   10     0.04023
       8   24    5   23     0.03788         7   37    8   24     0.03695
       6   32    8   10     0.03592         5   24    8   23     0.03541
       5   34    8   24     0.03531         5   29    8   10     0.03457
       4   31    8   10    -0.03408         8   23    5   24     0.03320
       5   23    8   10     0.03201         4   24    8   10     0.03062
*******************************************************************************
Triplet       B3G     ******************************************************
```

```
###   1-st  ###           ---  12th state in this spin multiplicity ---
    Total energy       in au =     -77.970458
    Correlation energy in au =       0.080414
    Excitation energy  in au =       0.351986    in eV =       9.578035
  *SINGLE EXCITATION
       7    9     0.83882         7   26     0.38415
       7   19    -0.18713         7   16     0.12183
       7   28    -0.11260         5   24     0.08860
       5   10     0.06360         7   13     0.06229
       7   32     0.05633         4   23     0.05188
       7   39     0.03392
  *DOUBLE EXCITATION
       8   27    5    9    -0.12674         8   18    5    9     0.08638
       8   35    7    9     0.07026         8   25    7    9    -0.06995
       8   36    5    9    -0.06292         8   27    5   26    -0.04850
       7   33    7    9    -0.03900         6   38    5    9    -0.03582
       7   29    5    9     0.03264         5   27    8    9    -0.03204
       6   29    4    9     0.03150
*****************************************************************************
Triplet       AU      ******************************************************
###   1-st  ###           ---   8th state in this spin multiplicity ---
    Total energy       in au =     -77.996916
    Correlation energy in au =       0.053956
    Excitation energy  in au =       0.325529    in eV =       8.858090
  *SINGLE EXCITATION
       8   12     0.87359         8   22     0.43015
       8   33     0.05266
  *DOUBLE EXCITATION
       8   25    8   12    -0.08714         8   35    8   12     0.08206
       7   33    8   12    -0.07141         5   29    8   12    -0.06619
       6   32    8   12    -0.06204         4   31    8   12     0.06113
       5   23    8   12    -0.05605         5   34    8   12     0.05124
       7   37    8   12     0.05062         8   25    8   22    -0.04030
       8   35    8   22     0.03789         4   24    8   12    -0.03381
       7   33    8   22    -0.03340         5   29    8   22    -0.03330
       7   22    8   12    -0.03144         4   31    8   22     0.03046
###   2-nd  ###           ---  19th state in this spin multiplicity ---
    Total energy       in au =     -77.949077
    Correlation energy in au =       0.101795
    Excitation energy  in au =       0.373367    in eV =      10.159846
  *SINGLE EXCITATION
       8   22    -0.86474         8   12     0.43418
       8   33    -0.11558         8   37     0.04128
  *DOUBLE EXCITATION
       8   25    8   22     0.08226         8   35    8   22    -0.07750
       7   33    8   22     0.06631         5   29    8   22     0.06610
       4   31    8   22    -0.06056         6   32    8   22     0.05998
       5   23    8   22     0.05243         7   37    8   22    -0.05040
       8   25    8   12    -0.04464         5   34    8   22    -0.04265
```

```
      8   35    8   12     0.04195         8   27    8   23    -0.03772
      7   33    8   12    -0.03603         5   29    8   12    -0.03238
      4   24    8   22     0.03144         6   32    8   12    -0.03105
      4   31    8   12     0.03012
*************************************************************************
Triplet       B1U     ****************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    Total energy       in au =     -78.156203
    Correlation energy in au =      -0.105331
    Excitation energy  in au =       0.166242    in eV =       4.523669
  *SINGLE EXCITATION
      8   27     0.69910         8   18    -0.66598
      8   36     0.17317         8   14    -0.11200
  *DOUBLE EXCITATION
      8   35    8   18    -0.03899         8   31    4   27     0.03728
      8   25    8   18     0.03405         8   35    8   27     0.03398
###   2-nd  ###           ---  11th state in this spin multiplicity ---
    Total energy       in au =     -77.991728
    Correlation energy in au =       0.059144
    Excitation energy  in au =       0.330717    in eV =       8.999263
  *SINGLE EXCITATION
      8   14     0.92626         8   27     0.26998
      8   18     0.13891         8   36     0.05091
  *DOUBLE EXCITATION
      8   25    8   14    -0.09311         8   35    8   14     0.08809
      7   33    8   14    -0.07590         5   29    8   14    -0.07002
      6   32    8   14    -0.06621         4   31    8   14     0.06464
      5   23    8   14    -0.05937         5   34    8   14     0.05451
      7   37    8   14     0.05333         7   22    8   14    -0.03640
      4   24    8   14    -0.03583
*************************************************************************
Triplet       B2U     ****************************************************
###   1-st  ###           ---  10th state in this spin multiplicity ---
    Total energy       in au =     -77.996247
    Correlation energy in au =       0.054625
    Excitation energy  in au =       0.326197    in eV =       8.876274
  *SINGLE EXCITATION
      8   15     0.86028         8   20     0.46110
  *DOUBLE EXCITATION
      8   25    8   15    -0.08698         8   35    8   15     0.08213
      7   33    8   15    -0.07018         5   29    8   15    -0.06360
      6   32    8   15    -0.06035         4   31    8   15     0.05915
      5   23    8   15    -0.05505         5   34    8   15     0.05083
      7   37    8   15     0.04862         8   35    8   20     0.04406
      8   25    8   20    -0.04383         7   33    8   20    -0.03625
      7   22    8   15    -0.03343         4   24    8   15    -0.03307
      5   29    8   20    -0.03234         6   32    8   20    -0.03097
      4   31    8   20     0.03022
###   2-nd  ###           ---  17th state in this spin multiplicity ---
```

```
    Total energy       in au =     -77.953447
    Correlation energy in au =       0.097425
    Excitation energy  in au =       0.368998    in eV =      10.040942
  *SINGLE EXCITATION
       8   20     0.86108         8   15    -0.46053
  *DOUBLE EXCITATION
       8   35    8   20     0.08168         8   25    8   20    -0.08143
       7   33    8   20    -0.06770         5   29    8   20    -0.06140
       6   32    8   20    -0.05862         4   31    8   20     0.05712
       5   23    8   20    -0.05147         5   34    8   20     0.05094
       8   25    8   15     0.04709         8   35    8   15    -0.04370
       7   37    8   20     0.03916         7   33    8   15     0.03778
       5   29    8   15     0.03480         6   32    8   15     0.03283
       4   31    8   15    -0.03218         4   24    8   20    -0.03167
       7   22    8   20    -0.03097
*******************************************************************************
Triplet       B3U     ****************************************************
###   1-st  ###           ---   2nd state in this spin multiplicity ---
    Total energy       in au =     -78.061817
    Correlation energy in au =      -0.010944
    Excitation energy  in au =       0.260628    in eV =       7.092048
  *SINGLE EXCITATION
       8    9     0.85918         8   26     0.38768
       8   16     0.17115         8   19    -0.15271
       8   28    -0.07434         8   13     0.06965
       8   21    -0.04834         8   39     0.03291
  *DOUBLE EXCITATION
       8   25    8    9    -0.07837         8   35    8    9     0.07786
       7   33    8    9    -0.06465         5   29    8    9    -0.06201
       6   32    8    9    -0.05997         4   31    8    9     0.05874
       5   34    8    9     0.03963         7   37    8    9     0.03893
       5   23    8    9    -0.03793         4   24    8    9    -0.03180
       8   27    8   24     0.03163
###   2-nd  ###           ---   7th state in this spin multiplicity ---
    Total energy       in au =     -77.999836
    Correlation energy in au =       0.051036
    Excitation energy  in au =       0.322609    in eV =       8.778624
  *SINGLE EXCITATION
       8   13    -0.70224         8   19    -0.57675
       8   16    -0.33475         8   28    -0.13181
  *DOUBLE EXCITATION
       8   25    8   13     0.07035         8   35    8   13    -0.06647
       7   33    8   13     0.05596         8   25    8   19     0.05454
       8   35    8   19    -0.05288         5   29    8   13     0.05256
       6   32    8   13     0.05025         4   31    8   13    -0.04126
       7   33    8   19     0.03521         5   23    8   13     0.03516
       8   25    8   16     0.03427         5   29    8   19     0.03421
       5   34    8   13    -0.03354         7   37    8   13    -0.03351
       8   35    8   16    -0.03277         4   31    8   19    -0.03264
```

```
      6   32    8   19     0.03258
###   3-rd  ###          ---   9th state in this spin multiplicity ---
    Total energy       in au =     -77.996880
    Correlation energy in au =       0.053992
    Excitation energy  in au =       0.325564    in eV =       8.859054
  *SINGLE EXCITATION
      8   16    -0.69682         8   21     0.53767
      8   13     0.37667         8    9     0.15729
      8   32     0.08078         8   26    -0.07856
      8   28    -0.04556         8   19    -0.04167
  *DOUBLE EXCITATION
      8   25    8   16     0.07042         8   35    8   16    -0.06752
      7   33    8   16     0.05513         8   35    8   21     0.04976
      6   32    8   16     0.04865         8   25    8   21    -0.04767
      5   29    8   16     0.04042         7   33    8   21    -0.04004
      4   31    8   16    -0.03948         8   25    8   13    -0.03774
      8   35    8   13     0.03538         5   23    8   16     0.03442
      5   34    8   16    -0.03344         7   37    8   16    -0.03170
      5   29    8   21    -0.03003
###   4-th  ###          ---  14th state in this spin multiplicity ---
    Total energy       in au =     -77.966879
    Correlation energy in au =       0.083993
    Excitation energy  in au =       0.355566    in eV =       9.675436
  *SINGLE EXCITATION
      8   19    -0.60614         8   13     0.49134
      8   26     0.38618         8    9    -0.36631
      8   28    -0.20533         8   16     0.12566
      8   21    -0.07855         8   39     0.03044
      8   32    -0.03024
  *DOUBLE EXCITATION
      8   25    8   19     0.05698         8   35    8   19    -0.05544
      8   25    8   13    -0.04993         8   35    8   13     0.04698
      8   25    8    9     0.04171         7   33    8   13    -0.03976
      8   35    8    9    -0.03839         5   29    8   13    -0.03601
      5   29    8   19     0.03518         7   33    8   19     0.03499
      6   32    8   13    -0.03479         4   31    8   19    -0.03374
      6   32    8   19     0.03336         7   33    8    9     0.03264
###   5-th  ###          ---  15th state in this spin multiplicity ---
    Total energy       in au =     -77.958898
    Correlation energy in au =       0.091974
    Excitation energy  in au =       0.363547    in eV =       9.892609
  *SINGLE EXCITATION
      8   21    -0.70755         8   16    -0.55962
      8   26     0.27185         8   19     0.19421
      8   32    -0.11843         8   28     0.11061
      8   13     0.08991
  *DOUBLE EXCITATION
      8   35    8   21    -0.06423         8   25    8   21     0.06052
      8   25    8   16     0.05995         8   35    8   16    -0.05432
```

```
      7   33    8   21     0.05285        7   33    8   16     0.04513
      6   32    8   16     0.04027        5   29    8   21     0.03874
      6   32    8   21     0.03829        4   31    8   21    -0.03826
      5   29    8   16     0.03370        4   31    8   16    -0.03300
      5   34    8   21    -0.03280        5   23    8   21     0.03233
================================================================
  STEP #DENS#  Density Calculation
================================================================
Transition density for SAC/SAC-CI (V)
Threshold for S2 operators (CThreDensULS2):  0.50D-02
Threshold for R1,R2 operators (CThreDensULR1):  0.10D+00
Left and right vectors are used. (ILEFT=1)
--------------------------------------------------------------------------------
Transition dipole moment of   triplet state from symmetry B1U    1-th state
--------------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
--------------------------------------------------------------------------------
   AG         1      3.5113      0.0000      0.0000      0.4700      0.0190
   AG         2      5.7308      0.0000      0.0000      0.2050      0.0059
   B1G        1      3.2837      0.0000      0.0000      0.0000      0.0000
   B1G        2      4.0282      0.0000      0.0000      0.0000      0.0000
   B1G        3      5.3723      0.0000      0.0000      0.0000      0.0000
   B2G        1      3.2757      0.5787      0.0000      0.0000      0.0269
   B2G        2      5.1399      0.1128      0.0000      0.0000      0.0016
   B2G        3      5.5225      0.3176      0.0000      0.0000      0.0136
   B3G        1      5.0544      0.0000     -0.0134      0.0000      0.0000
   AU         1      4.3344      0.0000      0.0000      0.0000      0.0000
   AU         2      5.6362      0.0000      0.0000      0.0000      0.0000
   B1U        1      0.0          Excitations are from this state.
   B1U        2      4.4756      0.0000      0.0000      0.0000      0.0000
   B2U        1      4.3526      0.0000      0.0000      0.0000      0.0000
   B2U        2      5.5173      0.0000      0.0000      0.0000      0.0000
   B3U        1      2.5684      0.0000      0.0000      0.0000      0.0000
   B3U        2      4.2550      0.0000      0.0000      0.0000      0.0000
   B3U        3      4.3354      0.0000      0.0000      0.0000      0.0000
   B3U        4      5.1518      0.0000      0.0000      0.0000      0.0000
   B3U        5      5.3689      0.0000      0.0000      0.0000      0.0000
--------------------------------------------------------------------------------
================================================================
  STEP #CIMX#  CI matrix elements          ### IONIZED STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Ionized   AG    CONVERGED
Solution for Ionized   B3G   CONVERGED
```

```
Solution for Ionized   B1U   CONVERGED
Solution for Ionized   B2U   CONVERGED
Solution for Ionized   B3U   CONVERGED
================================================================
  STEP #ULINTIA#  Unlinked integral for Ionized State (SAC-CI)
================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
================================================================
  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Ionized   AG    CONVERGED
Solution for Ionized   B3G   CONVERGED
Solution for Ionized   B1U   CONVERGED
Solution for Ionized   B2U   CONVERGED
Solution for Ionized   B3U   CONVERGED
************************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
************************************************
*******************************************************************************
CationDoublet AG      *******************************************************
###   1-st  ###           ---   3rd state in this spin multiplicity ---
    Total energy       in au =     -77.785425
    Correlation energy in au =       0.265447
    Excitation energy  in au =       0.537019    in eV =      14.613040
  *SINGLE EXCITATION
       6     0.96064
  *DOUBLE EXCITATION
       8   35    6     0.10571         8   27    4    -0.09931
       8   25    6    -0.09389         7   33    6    -0.07713
       6   32    6    -0.07504         8   18    4     0.06914
       5   34    6     0.06483         5   23    6    -0.05984
       5   29    6    -0.04713         8   36    4    -0.04562
       6   38    4    -0.04140         7   29    4     0.04047
       4   31    6     0.03973         7   28    7    -0.03832
       4   24    6    -0.03750         5   29    3     0.03610
       7   22    6    -0.03592         8   45    3     0.03564
       3   39    6    -0.03333         6   26    6    -0.03289
       6   32    3     0.03021
###   2-nd  ###           ---   6th state in this spin multiplicity ---
    Total energy       in au =     -77.430183
    Correlation energy in au =       0.620689
    Excitation energy  in au =       0.892262    in eV =      24.279675
  *SINGLE EXCITATION
       3     0.85448
  *DOUBLE EXCITATION
       8   27    4    -0.30200         4   27    8    -0.25019
```

```
      8   18    4     0.21433        8   28    8     0.19019
      4   18    8     0.17682        8   32    8    -0.13611
      8   36    4    -0.13587        8   35    3     0.11279
      4   36    8    -0.11059        8   19    8     0.09815
      8   25    3    -0.09599        8    9    8    -0.09148
      8   26    8    -0.08641        8   21    8    -0.08276
      5   29    6     0.08062        6   29    5     0.07843
      7   33    3    -0.07719        5   29    3    -0.07520
      7   28    7    -0.07389        8   45    6     0.07328
      6   32    3    -0.07285        7   30    5    -0.07075
      4   31    3     0.06733        5   34    3     0.06131
      6   32    6     0.06068        5   23    3    -0.05932
      6   45    8     0.05841        8   44    5     0.05576
      8   42    8     0.05152        5   28    5    -0.05031
      8   50    8     0.04893        6   38    4    -0.04408
      6   41    5    -0.04281        7   37    3     0.04223
      5   41    6    -0.04147        5   30    7    -0.03991
      8   47    7     0.03971        5   44    8     0.03918
      7   42    7    -0.03784        7   37    6    -0.03751
      4   38    6    -0.03694        7   33    6     0.03603
      4   24    3    -0.03536        7   43    5     0.03531
      4   40    3    -0.03517        3   35    8     0.03397
      7   47    8     0.03382        5   23    6     0.03359
      7   22    3    -0.03343        5   34    6    -0.03217
      8   17    3    -0.03002
*****************************************************************************
CationDoublet B3G     ****************************************************
###   1-st  ###           ---   2nd state in this spin multiplicity ---
    Total energy       in au =     -77.847191
    Correlation energy in au =       0.203681
    Excitation energy  in au =       0.475254    in eV =      12.932310
  *SINGLE EXCITATION
      7     0.96524
  *DOUBLE EXCITATION
      8   27    5    -0.13712        8   18    5     0.09431
      8   25    7    -0.08001        8   35    7     0.07908
      8   36    5    -0.06832        7   33    7    -0.05756
      6   38    5    -0.05195        7   29    5     0.05118
      5   23    7    -0.03719        6   29    4     0.03677
      7   30    4    -0.03527        5   34    7     0.03483
      7   41    5    -0.03340        7   22    7    -0.03334
      7   43    4     0.03295        8   44    4     0.03172
      5   27    8    -0.03138
*****************************************************************************
CationDoublet B1U     ****************************************************
###   1-st  ###           ---   5th state in this spin multiplicity ---
    Total energy       in au =     -77.608324
    Correlation energy in au =       0.442548
    Excitation energy  in au =       0.714121    in eV =      19.432208
```

```
  *SINGLE EXCITATION
       4     0.92289
  *DOUBLE EXCITATION
       8   27    6    -0.22591         8   18    6     0.16485
       8   27    3    -0.12353         6   27    8    -0.09182
       8   35    4     0.09106         8   36    6    -0.09069
       8   25    4    -0.08507         8   18    3     0.08466
       7   30    7    -0.08365         6   29    7     0.07820
       8   31    8     0.07799         7   29    6     0.07538
       6   18    8     0.06728         8   36    3    -0.06420
       5   28    7    -0.06261         7   33    4    -0.06222
       3   27    8    -0.06125         6   38    6    -0.05885
       7   43    7     0.05447         7   28    5    -0.04867
       6   41    7    -0.04156         5   34    4     0.03911
       8   45    4     0.03876         3   18    8     0.03829
       7   41    6    -0.03792         6   38    3    -0.03788
       5   42    7    -0.03782         7   42    5    -0.03774
       6   26    4    -0.03738         5   23    4    -0.03671
       4   24    4    -0.03583         6   32    4    -0.03412
       4   31    4     0.03293         4   38    4    -0.03209
       6   36    8    -0.03175         7   22    4    -0.03164
       8   38    8     0.03148         8   44    7     0.03141
       3   36    8    -0.03135         8   47    5     0.03130
*****************************************************************************
CationDoublet B2U     ******************************************************
###   1-st  ###           ---   4th state in this spin multiplicity ---
    Total energy       in au =     -77.730544
    Correlation energy in au =       0.320328
    Excitation energy  in au =       0.591901    in eV =      16.106438
  *SINGLE EXCITATION
       5     0.94090
  *DOUBLE EXCITATION
       8   27    7    -0.22861         8   18    7     0.16420
       8   36    7    -0.10054         8   35    5     0.08877
       8   25    5    -0.08699         7   27    8    -0.07313
       7   29    7     0.06447         7   33    5    -0.06427
       5   23    5    -0.05213         7   18    8     0.05196
       6   38    7    -0.04233         5   29    5    -0.04042
       5   34    5     0.03886         7   41    7    -0.03707
       6   32    5    -0.03599         7   22    5    -0.03471
       4   31    5     0.03346         8   44    3     0.03229
       7   36    8    -0.03128         4   24    5    -0.03108
*****************************************************************************
CationDoublet B3U     ******************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    Total energy       in au =     -77.942703
    Correlation energy in au =       0.108169
    Excitation energy  in au =       0.379742    in eV =      10.333293
  *SINGLE EXCITATION
```

```
      8     0.97517
  *DOUBLE EXCITATION
      8   25    8    -0.09815         8   35    8     0.09234
      7   33    8    -0.07875         5   29    8    -0.07181
      6   32    8    -0.06918         4   31    8     0.06669
      5   23    8    -0.06208         5   34    8     0.05736
      7   37    8     0.05502         7   22    8    -0.04792
      4   24    8    -0.03784         8   17    8    -0.03226
      4   27    3    -0.03017
==============================================================
  STEP #SATEI#  Monopole Intensity Calculation
==============================================================
Symmetry  State     I.P.        Intensity
-------------------------------------------
AG          1      14.613       0.92296
            2      24.280       0.73015
-------------------------------------------
B3G         1      12.932       0.93168
-------------------------------------------
B1U         1      19.432       0.85172
-------------------------------------------
B2U         1      16.106       0.88529
-------------------------------------------
B3U         1      10.333       0.95096
-------------------------------------------
==============================================================
  STEP #DENS#  Density Calculation
==============================================================
Transition density for SAC/SAC-CI (V)
Threshold for S2 operators (CThreDensULS2):  0.50D-02
Threshold for R1,R2 operators (CThreDensULR1):  0.10D+00
Left and right vectors are used. (ILEFT=1)
-----------------------------------------------------------------------------------
Transition dipole moment of   ionized state from symmetry B3U    1-th state
-----------------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
-----------------------------------------------------------------------------------
   AG         1      4.2797      0.1152      0.0000      0.0000      0.0014
   AG         2     13.9464      0.3958      0.0000      0.0000      0.0535
   B3G        1      2.5990      0.0000      0.0000      0.0000      0.0000
   B1U        1      9.0989      0.0000      0.0000      0.0000      0.0000
   B2U        1      5.7731      0.0000      0.0000      0.0000      0.0000
   B3U        1      0.0          Excitations are from this state.
-----------------------------------------------------------------------------------
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.

*******************************************************************
```

```
          Population analysis using the SCF density.

***********************************************************************

Orbital symmetries:
      Occupied  (AG) (B1U) (AG) (B1U) (B2U) (AG) (B3G) (B3U)
      Virtual   (AG) (B1U) (B2U) (B3G) (AG) (B2G) (B1G) (AG) (B3U)
                (B2G) (AG) (B1G) (AG) (B3G) (B2U) (B1U) (B3U)
                (AG) (B2G) (AG) (B2U) (B1U) (B1U) (AG) (B3G) (B2U)
                (B3U) (B2G) (B3G) (B1U) (AG) (B1U) (B2U) (AG)
                (B1U) (B1G) (B3U) (B3G) (AU) (AG) (B3G) (AG) (B2U)
                (B1U) (B2G) (B2U) (B3U) (B1G) (B1U) (B2G) (AU)
                (AG) (B3G) (B1U) (AG) (B2U) (B1U) (B3G) (AG) (B1U)
The electronic state is 1-AG.
Alpha  occ. eigenvalues --  -11.24168 -11.24006  -1.03312  -0.79239  -0.64303
Alpha  occ. eigenvalues --   -0.58530  -0.50819  -0.37482
Alpha virt. eigenvalues --    0.03169   0.03468   0.03508   0.03551   0.03554
Alpha virt. eigenvalues --    0.03594   0.03658   0.03681   0.03845   0.10243
Alpha virt. eigenvalues --    0.11738   0.12373   0.12463   0.12670   0.15159
Alpha virt. eigenvalues --    0.15506   0.16761   0.18701   0.19263   0.36642
Alpha virt. eigenvalues --    0.36675   0.39651   0.42002   0.50170   0.56519
Alpha virt. eigenvalues --    0.63239   0.67847   0.68330   0.69338   0.87168
Alpha virt. eigenvalues --    0.96023   1.13895   1.20076   1.32574   1.33696
Alpha virt. eigenvalues --    1.53533   1.56517   1.60212   1.67370   1.96825
Alpha virt. eigenvalues --    2.07478   2.10752   2.11875   2.22033   2.24784
Alpha virt. eigenvalues --    2.43427   2.48609   2.56965   2.61687   2.78096
Alpha virt. eigenvalues --    2.84691   2.94824   2.99706   3.21255   3.36390
Alpha virt. eigenvalues --    3.51834   3.70422   3.93431  24.04900  24.38610
         Condensed to atoms (all electrons):
              1          2          3          4          5          6
    1  H    0.527370   0.412861  -0.038682  -0.005602   0.002285  -0.030002
    2  C    0.412861   4.861946   0.619506  -0.038682  -0.038682   0.412861
    3  C   -0.038682   0.619506   4.861946   0.412861   0.412861  -0.038682
    4  H   -0.005602  -0.038682   0.412861   0.527370  -0.030002   0.002285
    5  H    0.002285  -0.038682   0.412861  -0.030002   0.527370  -0.005602
    6  H   -0.030002   0.412861  -0.038682   0.002285  -0.005602   0.527370
    7  Bq   0.006713   0.002089   0.002089   0.006713   0.006713   0.006713
              7
    1  H    0.006713
    2  C    0.002089
    3  C    0.002089
    4  H    0.006713
    5  H    0.006713
    6  H    0.006713
    7  Bq   0.005399
Mulliken atomic charges:
              1
    1  H    0.125057
```

```
    2  C   -0.231900
    3  C   -0.231900
    4  H    0.125057
    5  H    0.125057
    6  H    0.125057
    7  Bq  -0.036428
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  H    0.000000
    2  C    0.018214
    3  C    0.018214
    4  H    0.000000
    5  H    0.000000
    6  H    0.000000
    7  Bq  -0.036428
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    83.5302
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     0.0000    Y=     0.0000    Z=     0.0000  Tot=     0.0000
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=   -16.2640   YY=   -12.2863   ZZ=   -12.1376
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -2.7013   YY=     1.2763   ZZ=     1.4250
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=     0.0000  YYY=     0.0000  ZZZ=     0.0000  XYY=     0.0000
 XXY=     0.0000  XXZ=     0.0000  XZZ=     0.0000  YZZ=     0.0000
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=   -21.6535 YYYY=   -27.0739 ZZZZ=   -68.5119 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=    -8.8502 XXZZ=   -16.1757 YYZZ=   -13.1232
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 3.324999423628D+01 E-N=-2.476162242765D+02  KE= 7.785168423628D+01
Symmetry AG   KE= 3.748532068494D+01
Symmetry B1G  KE= 9.684633491136D-34
Symmetry B2G  KE= 3.251299784892D-32
Symmetry B3G  KE= 2.083198795373D+00
Symmetry AU   KE= 1.257391018236D-33
Symmetry B1U  KE= 3.454340302188D+01
Symmetry B2U  KE= 1.827961283940D+00
Symmetry B3U  KE= 1.911800450144D+00

Test job not archived.
1¥1¥GINC-MIRAI86¥SP¥RSACCI¥Gen¥C2H4N1¥MASAHIRO¥31-Jul-2004¥0¥¥# SAC-CI
(LEVELTWO, SINGLET=(NSTATE=(2,3,3,1,2,2,2,5)), TRIPLET=(NSTATE=(2,3,3,
```

```
1,2,2,2,5)), CATIONDOUBLET=(NSTATE=(2,0,0,1,0,1,1,1))) /GEN MASSAGE SY
MM=ON TEST¥¥Gaussian Test Job 635 (Part 2): SAC-CI SD-R LevelTwo calcu
lations for ethylene.¥¥0,1¥H¥C,1,1.0868¥C,2,1.3391,1,121.28¥H,3,1.0868
,2,121.28,1,0.,0¥H,3,1.0868,2,121.28,1,180.,0¥H,2,1.0868,3,121.28,4,18
0.,0¥Bq,2,0.66955,1,121.28,4,0.,0¥¥Version=AI64T-G03RevC.02¥State=1-AG
¥HF=-78.050872¥RMSD=3.635e-09¥PG=D02H [O(N1),C2"(C1.C1),SG(H4)]¥¥@


THE HURRIEDER I GO, THE BEHINDER I GET.
Job cpu time:  0 days  0 hours  4 minutes 59.4 seconds.
File lengths (MBytes):  RWF=    579 Int=      0 D2E=      0 Chk=     14 Scr=     48
Normal termination of Gaussian 03 at Sat Jul 31 11:57:47 2004.
Initial command:
/work/g03.C02/g03/l1.exe /work/g03.C02/inputs/Gau-113434.inp -scrdir=/work/g03.C02/inputs/
Entering Link 1 = /work/g03.C02/g03/l1.exe PID=    113480.

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H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,
A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

****************************************
Gaussian 03:  AI64T-G03RevC.02 12-Jun-2004
               31-Jul-2004
****************************************
%mem=12mw
---------------------------------------------------------------------------
# SAC-CI(LevelThree, Singlet=(NState=(2,3,3,1,2,2,2,5)), Triplet=(NSta
te=(2,3,3,1,2,2,2,5)), CationDoublet=(NState=(2,0,0,1,0,1,1,1))) /Gen
Massage Symm=On test
---------------------------------------------------------------------------
1/38=1/1;
2/15=-1,17=6,18=5,40=1/2;
```

This calculation requires "LevelThree" accuracy in the perturbation selection.

```
3/5=7,10=10,11=9,16=1,25=1,30=1,36=2/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=5,9=30000,10=1,40=1,42=2/1,4;
9//23;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;
---------------------------------------------------------------------
Gaussian Test Job 635 (Part 3): SAC-CI SD-R LevelThree calculations fo
r ethylene
---------------------------------------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
H1
C2                  1    r1
C3                  2    r2       1    a1
H4                  3    r1       2    a1       1     0.       0
H5                  3    r1       2    a1       1     180.     0
H6                  2    r1       3    a1       4     180.     0
N7                  2    r22      1    a1       4     0.       0
      Variables:
 r1                   1.0868
 r2                   1.3391
 a1                 121.28
 r22                  0.66955

                        Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          1           0        0.000000    0.000000    0.000000
   2          6           0        0.000000    0.000000    1.086800
   3          6           0        1.144449    0.000000    1.782089
   4          1           0        2.108977    0.000000    1.281270
   5          1           0        1.144449    0.000000    2.868889
   6          1           0       -0.964528    0.000000    1.587619
   7          7           0        0.572224    0.000000    1.434444
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  H    0.000000
    2  C    1.086800   0.000000
    3  C    2.117924   1.339100   0.000000
    4  H    2.467678   2.117924   1.086800   0.000000
    5  H    3.088735   2.117924   1.086800   1.857646   0.000000
    6  H    1.857646   1.086800   2.117924   3.088735   2.467678
    7  N    1.544368   0.669550   0.669550   1.544368   1.544368
                  6          7
```

```
    6  H    0.000000
    7  N    1.544368   0.000000
Stoichiometry    C2H4N
Framework group  D2H[O(N),C2"(C.C),SG(H4)]
Deg. of freedom     3
Full point group                 D2H     NOp   8
Largest Abelian subgroup         D2H     NOp   8
Largest concise Abelian subgroup D2      NOp   4
                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          1            0        0.000000    0.928823    1.233839
   2          6            0        0.000000    0.000000    0.669550
   3          6            0        0.000000    0.000000   -0.669550
   4          1            0        0.000000    0.928823   -1.233839
   5          1            0        0.000000   -0.928823   -1.233839
   6          1            0        0.000000   -0.928823    1.233839
   7          7            0        0.000000    0.000000    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    145.3135944     29.9107742     24.8050094
General basis read from cards:  (5D, 7F)
The nuclear charge for atom    7 has been changed to Z=  0   0.000000
There are    18 symmetry adapted basis functions of AG  symmetry.
There are     4 symmetry adapted basis functions of B1G symmetry.
There are     6 symmetry adapted basis functions of B2G symmetry.
There are     9 symmetry adapted basis functions of B3G symmetry.
There are     2 symmetry adapted basis functions of AU  symmetry.
There are    14 symmetry adapted basis functions of B1U symmetry.
There are     9 symmetry adapted basis functions of B2U symmetry.
There are     6 symmetry adapted basis functions of B3U symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   68 basis functions,   108 primitive gaussians,    72 cartesian basis functions
    8 alpha electrons        8 beta electrons
      nuclear repulsion energy        33.2499942363 Hartrees.
NAtoms=    7 NActive=    7 NUniq=    3 SFac= 5.66D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    68 RedAO= T  NBF=    18     4     6     9     2    14     9     6
NBsUse=    68 1.00D-06 NBFU=    18     4     6     9     2    14     9     6
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.13D-02 ExpMax= 4.23D+03 ExpMxC= 6.35D+02 IAcc=3 IRadAn=         5 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=         5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Warning:  off-atom basis functions, so minimal bfn integration tests in XC quadrature.
Initial guess orbital symmetries:
      Occupied  (AG) (B1U) (AG) (B1U) (B2U) (AG) (B3G) (B3U)
```

```
      Virtual   (B2G) (AG) (B2U) (B1U) (B3U) (AG) (B3G) (AG) (B2G)
                (B1G) (AG) (B2U) (B1U) (B3G) (AG) (B1G) (AG) (B3U)
                (B2G) (B2U) (B1U) (AG) (B1U) (AG) (B3G) (B2U)
                (B2G) (B3U) (B1U) (B3G) (AG) (B1U) (B2U) (AG)
                (B1U) (B1G) (B3U) (B3G) (AU) (AG) (AG) (B3G) (B2U)
                (B1U) (B2G) (B2U) (B3U) (B1U) (B1G) (B2G) (AU)
                (AG) (B3G) (B1U) (AG) (B2U) (B1U) (B3G) (AG) (B1U)
The electronic state of the initial guess is 1-AG.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=     4505542.
SCF Done:  E(RHF) =  -78.0508720221     A.U. after    9 cycles
           Convg  =    0.3635D-08             -V/T =  2.0026
           S**2   =   0.0000
ExpMin= 1.13D-02 ExpMax= 4.23D+03 ExpMxC= 6.35D+02 IAcc=3 IRadAn=        5 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=        5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Warning:  off-atom basis functions, so minimal bfn integration tests in XC quadrature.
Range of M.O.s used for correlation:     3    68
NBasis=    68 NAE=     8 NBE=     8 NFC=     2 NFV=     0
NROrb=     66 NOA=     6 NOB=     6 NVA=    60 NVB=    60
-----------------------------------------------------------------------
#######################################################################
-----------------------------------------------------------------------
              SAC/SAC-CI Program Combined with GAUSSIAN
                          for Calculating
        Ground, Excited, Ionized, and Electron-Attached States
                                and
             Singlet, Doublet, Triplet, Quartet, Quintet,
                    Sextet, and Septet Spin States
                                and
                  Their Analytical Energy Gradients
                         coded originally by
                          Hiroshi Nakatsuji
                           and extended by
 H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa,
      M. Ishida, T. Nakajima, Y. Honda, O. Kitao, and H. Nakai
                                at
                  Department of Hydrocarbon Chemistry,
                Division of Molecular Engineering, and
     Department of Synthetic Chemistry & Biological Chemistry,
                   Graduate School of Engineering,
                          Kyoto University,
                        Kyoto 606-8501, Japan
-----------------------------------------------------------------------
#######################################################################
-----------------------------------------------------------------------
```

```
No. of INTEGRALS =    324236 NBLK =       202 KOUNT =      1036
##############################################################################
    Singles-Doubles (SD) SAC/SAC-CI  (SAC-CI SD-R)
##############################################################################
================================================================
  STEP #PRES#  Generation of Linked Operators and Selection
================================================================
== States to be calculated ==
           AG   B1G  B2G  B3G  AU   B1U  B2U  B3U
SINGLET    Yes  Yes  Yes  Yes  Yes  Yes  Yes  Yes
TRIPLET    Yes  Yes  Yes  Yes  Yes  Yes  Yes  Yes
IONIZED    Yes  Yes  Yes  Yes  Yes  Yes  Yes  Yes
ANIONIZED  No   No   No   No   No   No   No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  3,  3,  3,  1,  2,  2,  2,  5)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
TRIPLET STATE
 Number of States  Triplet      =(  2,  3,  3,  1,  2,  2,  2,  5)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreR2 (Lambda_E)=  0.100D-06(au)
IONIZED STATE
 Number of States  CationDoublet=(  2,  0,  0,  1,  0,  1,  1,  1)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreR2 (Lambda_E)=  0.100D-06(au)
****************************
        SINGLET STATE
****************************
----------------------------------------------------------------
LINKED OPERATORS FOR SAC:    SYMMETRY = AG  GROUND STATE
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            63        9024         9087
    AFTER             63        5051         5115
----------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AG  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.296334
       8 ->  17     0.94023        8 ->  25     0.32851
    ##   2-nd state ##       energy (au) =       0.380223
       8 ->  25     0.92052        8 ->  17    -0.33907
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            63        9024         9087
    AFTER             63        3535         3599
----------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1G EXCITED STATE
```

Compared with the results by the "LevelOne" and "LevelTwo" thresholds in the former inputs, the number of selected operators increased. The same is for all the states.

```
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.281843
       8 ->  11     0.86335        8 ->  23     0.48630
       8 ->  29     0.10227
    ##   2-nd state ##       energy (au) =       0.341571
       7 ->  18     0.72120        7 ->  27    -0.64239
       7 ->  14     0.14162        8 ->  23     0.11167
       7 ->  36    -0.11143        8 ->  11    -0.11010
    ##   3-th state ##       energy (au) =       0.356963
       8 ->  23     0.82116        8 ->  11    -0.49204
       8 ->  29     0.19651        8 ->  34    -0.12686
       7 ->  18    -0.12591        7 ->  27     0.10502
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            29        7364         7393
    AFTER             29        4205         4234
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.287373
       8 ->  10     0.91243        8 ->  24     0.39911
    ##   2-nd state ##       energy (au) =       0.369257
       8 ->  24     0.81584        8 ->  10    -0.38382
       6 ->  27    -0.27427        6 ->  18     0.26566
       8 ->  31    -0.17400
    ##   3-th state ##       energy (au) =       0.376304
       6 ->  27     0.63715        6 ->  18    -0.62072
       8 ->  24     0.37166        6 ->  36     0.15588
       8 ->  10    -0.14036        6 ->  14    -0.10387
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            35        7484         7519
    AFTER             35        4385         4420
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.386987
       7 ->   9     0.87379        7 ->  26     0.37236
       7 ->  19    -0.16572        7 ->  16     0.14314
       5 ->  24     0.11788
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            53        8708         8761
    AFTER             53        3900         3953
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AU  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.320962
       8 ->  12     0.90268        8 ->  22     0.42641
    ##   2-nd state ##       energy (au) =       0.368854
       8 ->  22     0.89326        8 ->  12    -0.43030
       8 ->  33     0.12187
```

```
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            27        7356         7383
    AFTER             27        2080         2107
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.284181
       8 ->  18     0.82474        8 ->  27    -0.40146
       8 ->  14     0.33925
    ##   2-nd state ##       energy (au) =       0.331060
       8 ->  14     0.91523        8 ->  27     0.34202
       8 ->  18    -0.18352
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            61        8836         8897
    AFTER             61        3951         4012
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.320792
       8 ->  15     0.88807        8 ->  20     0.45915
    ##   2-nd state ##       energy (au) =       0.364234
       8 ->  20     0.88703        8 ->  15    -0.45967
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            55        8716         8771
    AFTER             55        1345         1400
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.260350
       8 ->   9     0.89702        8 ->  26     0.35048
       8 ->  16     0.17828        8 ->  19    -0.16415
    ##   2-nd state ##       energy (au) =       0.315645
       8 ->  13     0.72791        8 ->  19     0.57881
       8 ->  16     0.34382        8 ->  28     0.11322
    ##   3-th state ##       energy (au) =       0.319844
       8 ->  16     0.77242        8 ->  21    -0.48071
       8 ->  13    -0.38277        8 ->   9    -0.14211
    ##   4-th state ##       energy (au) =       0.348811
       8 ->  19     0.65807        8 ->  13    -0.49993
       8 ->   9     0.34671        8 ->  26    -0.34490
       8 ->  28     0.20148        8 ->  16    -0.17875
    ##   5-th state ##       energy (au) =       0.361679
       8 ->  21     0.82835        8 ->  16     0.46809
       8 ->  26    -0.20355        8 ->  19    -0.13967
       8 ->  13    -0.13875
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            37        7492         7529
    AFTER             37        3352         3389
****************************
```

```
        TRIPLET STATE
****************************
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AG  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.284276
       8 ->  17     0.86842        8 ->  25     0.48460
    ##   2-nd state ##       energy (au) =       0.363288
       8 ->  25     0.85196        8 ->  17    -0.49556
       8 ->  35    -0.15070
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            63       12189        12252
    AFTER             63        2666         2729
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.278966
       8 ->  11     0.83989        8 ->  23     0.51633
       8 ->  29     0.12821
    ##   2-nd state ##       energy (au) =       0.316463
       7 ->  18     0.70581        7 ->  27    -0.67742
       7 ->  14     0.12567        7 ->  36    -0.12532
    ##   3-th state ##       energy (au) =       0.352620
       8 ->  23     0.79138        8 ->  11    -0.53814
       8 ->  29     0.24969        8 ->  34    -0.13223
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            29       10500        10529
    AFTER             29        5749         5778
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.283348
       8 ->  10     0.88446        8 ->  24     0.44379
       8 ->  31    -0.13053
    ##   2-nd state ##       energy (au) =       0.347308
       6 ->  27     0.69974        6 ->  18    -0.64978
       6 ->  36     0.18078        8 ->  10     0.10859
       8 ->  24    -0.10797        6 ->  14    -0.10124
    ##   3-th state ##       energy (au) =       0.364354
       8 ->  24     0.84635        8 ->  10    -0.45313
       8 ->  31    -0.21638        6 ->  27     0.11741
       6 ->  18    -0.10643
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            35       10602        10637
    AFTER             35        5897         5932
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.370044
```

```
      7 ->   9     0.77647        7 ->  26     0.44073
      7 ->  19    -0.21913        7 ->  28    -0.17447
      5 ->  24     0.17377        5 ->  10     0.11183
      7 ->  16     0.11173
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            53       12222        12275
    AFTER             53        6074         6127
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AU  EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.320525
      8 ->  12     0.89588        8 ->  22     0.43915
    ##   2-nd state ##       energy (au) =       0.367583
      8 ->  22     0.88376        8 ->  12    -0.44423
      8 ->  33     0.13093
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            27       10506        10533
    AFTER             27        2924         2951
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.129560
      8 ->  27     0.71782        8 ->  18    -0.66032
      8 ->  36     0.17938        8 ->  14    -0.10220
    ##   2-nd state ##       energy (au) =       0.324207
      8 ->  14     0.93866        8 ->  27     0.28541
      8 ->  18     0.18242
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            61       12318        12379
    AFTER             61        3078         3139
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.319743
      8 ->  15     0.86916        8 ->  20     0.49394
    ##   2-nd state ##       energy (au) =       0.361471
      8 ->  20     0.86729        8 ->  15    -0.49439
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            55       12240        12295
    AFTER             55        1728         1783
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.252381
      8 ->   9     0.85547        8 ->  26     0.42815
      8 ->  16     0.19023        8 ->  19    -0.16184
    ##   2-nd state ##       energy (au) =       0.313559
      8 ->  16     0.62658        8 ->  19     0.54898
      8 ->  13     0.40646        8 ->  21    -0.32387
```

```
      8 ->  28     0.15678
   ##   3-th state ##       energy (au) =       0.315979
      8 ->  13     0.68320        8 ->  21     0.49464
      8 ->  16    -0.38839        8 ->  19     0.26803
      8 ->   9     0.20236        8 ->  26    -0.11168
      8 ->  32     0.10498
   ##   4-th state ##       energy (au) =       0.345015
      8 ->  13     0.53277        8 ->  19    -0.50357
      8 ->  26     0.47087        8 ->   9    -0.39931
      8 ->  21    -0.20178        8 ->  28    -0.17378
   ##   5-th state ##       energy (au) =       0.350851
      8 ->  16     0.64554        8 ->  21     0.60356
      8 ->  19    -0.35868        8 ->  26    -0.20475
      8 ->  28    -0.16720        8 ->  32     0.11453
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            37       10593        10630
    AFTER             37        4482         4519
****************************
       IONIZED STATE
****************************
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = AG  EXCITED STATE
  #SECI# Main reference configuration and coefficient
   ##   1-st state ##       energy (au) =       0.585304
      6     1.00000
   ##   2-nd state ##       energy (au) =       1.033118
      3     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             2         332          334
    AFTER              2         328          330
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE
  #SECI# Main reference configuration and coefficient
   ##   1-st state ##       energy (au) =       0.508192
      7     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1         312          313
    AFTER              1         298          299
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE
  #SECI# Main reference configuration and coefficient
   ##   1-st state ##       energy (au) =       0.792389
      4     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1         328          329
    AFTER              1         311          312
------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE
  #SECI# Main reference configuration and coefficient
```

```
    ##   1-st state ##       energy (au) =       0.643034
       5     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1         316         317
    AFTER              1         296         297
-----------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.374824
       8     1.00000
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             1         228         229
    AFTER              1         209         210
=============================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
=============================================================
=============================================================
  STEP #DIAGCI#  Solution of SDCI
=============================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   AG    CONVERGED
Solution for Singlet   AG    CONVERGED
Solution for Singlet   B1G   CONVERGED
Solution for Singlet   B2G   CONVERGED
Solution for Singlet   B3G   CONVERGED
Solution for Singlet   AU    CONVERGED
Solution for Singlet   B1U   CONVERGED
Solution for Singlet   B2U   CONVERGED
Solution for Singlet   B3U   CONVERGED
=============================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
=============================================================
Threshold for S2 operator (CThreULS2G) 0.500D-02
=============================================================
  STEP #SAC#  Solution of SAC equation
=============================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-05
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Solution for SAC equation converged
*********************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*********************************************
HF ENERGY     =     -78.050872 (AU)
SAC-NV  ENERGY=      -0.283870 (AU)
TOTAL ENERGY  =     -78.334742 (AU)
```

```
SAC-NV  coefficients (|C|>=0.03)
*SINGLE EXCITATION
*DOUBLE EXCITATION
       8   27    8   18      0.11751         8   27    8   27     -0.08375
       8   36    8   27     -0.07695         8   36    8   18      0.05061
       8   27    6   38     -0.04771         8   18    8   18     -0.04190
       8   36    6   38     -0.03934         8   27    3   31      0.03237
       8   18    6   38      0.03005
Hartree-Fock configuration   1.00000
=====================================================================
  STEP #ULINTS#  Unlinked integral for Singlet Excited State (SAC-CI)
=====================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
=================================================================
  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
=================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   AG    CONVERGED
Solution for Singlet   B1G   CONVERGED
Solution for Singlet   B2G   CONVERGED
Solution for Singlet   B3G   CONVERGED
Solution for Singlet   AU    CONVERGED
Solution for Singlet   B1U   CONVERGED
Solution for Singlet   B2U   CONVERGED
Solution for Singlet   B3U   CONVERGED
***********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
***********************************************
*******************************************************************************
Singlet       AG      ******************************************************
###   1-st  ###           ---   5th state in this spin multiplicity ---
    Total energy       in au =     -78.032563
    Correlation energy in au =       0.018309
    Excitation energy  in au =       0.302180    in eV =       8.222723
  *SINGLE EXCITATION
       8   17     0.91474         8   25     0.32815
  *DOUBLE EXCITATION
       8   25    8   17    -0.10479         8   35    8   17     0.08730
       8   17    7   33    -0.07089         8   17    5   29    -0.06388
       8   17    6   32    -0.06215         8   17    4   31     0.06001
       8   17    5   23    -0.05555         8   17    5   34     0.05271
       8   17    7   37     0.04882         8   36    8   27     0.04417
       8   27    8   27     0.04003         8   17    4   24    -0.03357
       8   17    7   22    -0.03293         8   25    8   25    -0.03270
       8   35    8   25     0.03007
###   2-nd  ###           ---  20th state in this spin multiplicity ---
    Total energy       in au =     -77.947539
```

```
    Correlation energy in au =       0.103333
    Excitation energy  in au =       0.387204    in eV =      10.536345
  *SINGLE EXCITATION
       8   25     0.89837         8   17    -0.33805
       8   35    -0.09209         7   22    -0.07332
       6    9    -0.05784         7   33    -0.03098
  *DOUBLE EXCITATION
       8   25    8   25    -0.09032         8   35    8   25     0.08952
       8   36    8   27     0.07549         8   25    7   33    -0.06199
       8   27    8   27     0.05865         8   27    8   18    -0.05574
       8   25    6   32    -0.05366         8   25    5   29    -0.05363
       8   25    4   31     0.05219         8   36    8   18    -0.04720
       8   25    5   34     0.03905         8   25    5   23    -0.03799
       8   25    7   37     0.03445         8   35    8   17    -0.03136
       8   17    7   33     0.03006
*****************************************************************************
Singlet       B1G     ******************************************************
###   1-st  ###           ---   2nd state in this spin multiplicity ---
    Total energy       in au =     -78.045245
    Correlation energy in au =       0.005627
    Excitation energy  in au =       0.289498    in eV =       7.877630
  *SINGLE EXCITATION
       8   11     0.85284         8   23     0.45899
       8   29     0.08630         8   34    -0.07015
       7   18     0.03944         7   27    -0.03724
  *DOUBLE EXCITATION
       8   25    8   11    -0.08360         8   35    8   11     0.07841
       8   11    7   33    -0.06582         8   11    5   29    -0.06009
       8   11    6   32    -0.05802         8   11    4   31     0.05690
       8   11    5   23    -0.05250         8   11    5   34     0.04154
       8   25    8   23    -0.04043         8   11    7   37     0.03878
       8   35    8   23     0.03609         8   11    4   24    -0.03145
       8   11    7   22    -0.03129         8   33    8   27     0.03088
###   2-nd  ###           ---  10th state in this spin multiplicity ---
    Total energy       in au =     -78.006130
    Correlation energy in au =       0.044742
    Excitation energy  in au =       0.328613    in eV =       8.942001
  *SINGLE EXCITATION
       7   18    -0.71488         7   27     0.61559
       7   14    -0.14505         7   36     0.11264
       8   11     0.08842         8   29    -0.05890
       8   23    -0.03255
  *DOUBLE EXCITATION
       8   27    5   18     0.11855         8   27    5   27    -0.11068
       8   18    5   18    -0.09228         8   18    5   27     0.09153
       8   36    5   18     0.03968         7   30    4   18     0.03557
       7   30    4   27    -0.03555         8   35    7   36    -0.03439
       7   29    5   18    -0.03272         7   43    4   27     0.03229
       7   43    4   18    -0.03192         6   38    5   18     0.03181
```

```
      7   29    5   27     0.03157         8   36    5   27    -0.03053
###   3-rd  ###          ---  14th state in this spin multiplicity ---
    Total energy       in au =     -77.967827
    Correlation energy in au =       0.083045
    Excitation energy  in au =       0.366916    in eV =       9.984288
  *SINGLE EXCITATION
      8   23     0.82592         8   11    -0.46628
      8   29     0.18234         8   34    -0.12505
      7   18    -0.06717         7   27     0.04569
  *DOUBLE EXCITATION
      8   25    8   23    -0.07468         8   35    8   23     0.06882
      8   23    7   33    -0.05571         8   23    5   29    -0.05268
      8   25    8   11     0.04977         8   35    8   11    -0.04755
      8   33    8   27     0.04433         8   23    4   31     0.04280
      8   23    5   23    -0.04048         8   11    7   33     0.04007
      8   23    6   32    -0.04004         8   23    5   34     0.03677
      8   11    6   32     0.03607         8   11    5   29     0.03589
      8   11    4   31    -0.03375         8   23    7   37     0.03322
      8   11    5   23     0.03113
*************************************************************************
Singlet       B2G     ******************************************************
###   1-st  ###          ---   3rd state in this spin multiplicity ---
    Total energy       in au =     -78.044369
    Correlation energy in au =       0.006503
    Excitation energy  in au =       0.290374    in eV =       7.901468
  *SINGLE EXCITATION
      8   10     0.87547         8   24     0.41474
      8   31    -0.09076
  *DOUBLE EXCITATION
      8   25    8   10    -0.08538         8   35    8   10     0.08014
      8   10    7   33    -0.06797         8   10    5   29    -0.06674
      8   10    6   32    -0.06301         8   10    4   31     0.06141
      8   10    5   23    -0.05283         8   10    7   37     0.04993
      8   10    5   34     0.04118         8   27    8    9     0.04115
      8   26    8   18    -0.04041         8   27    8   26     0.03983
      8   25    8   24    -0.03693         8   10    4   24    -0.03420
      8   35    8   24     0.03315         8   10    7   22    -0.03274
      8   24    5   29    -0.03264
###   2-nd  ###          ---  17th state in this spin multiplicity ---
    Total energy       in au =     -77.962391
    Correlation energy in au =       0.088481
    Excitation energy  in au =       0.372351    in eV =      10.132197
  *SINGLE EXCITATION
      8   24     0.74937         8   10    -0.39307
      6   18     0.31592         6   27    -0.29440
      8   31    -0.17964         6   36    -0.06568
      6   14     0.05615         8   30    -0.05189
  *DOUBLE EXCITATION
      8   25    8   24    -0.06893         8   27    8   26     0.06584
```

```
      8   35    8   24     0.06374         8   26    8   18    -0.05662
      8   24    5   29    -0.05621         8   24    7   33    -0.05276
      8   24    6   32    -0.05209         8   24    4   31     0.05170
      8   27    4   27     0.04616         8   27    4   18    -0.04373
      8   25    8   10     0.04204         8   35    8   10    -0.04021
      8   24    7   37     0.03384         8   24    5   23    -0.03363
      8   10    7   33     0.03362         8   24    5   34     0.03186
      8   27    8    9     0.03160         8   24    4   24    -0.03129
      8   32    8   27     0.03099
###   3-rd  ###           ---  19th state in this spin multiplicity ---
    Total energy       in au =     -77.954983
    Correlation energy in au =       0.095889
    Excitation energy  in au =       0.379759    in eV =      10.333776
  *SINGLE EXCITATION
      6   18     0.62154         6   27    -0.57512
      8   24    -0.41016         8   10     0.17261
      6   36    -0.12839         6   14     0.11758
      3   27     0.05451         8   31     0.03481
      3   18    -0.03309
  *DOUBLE EXCITATION
      8   27    4   18    -0.06475         8   27    4   27     0.05627
      8   18    4   18     0.05401         8   18    4   27    -0.05083
      8   25    8   24     0.03929         8   35    8   24    -0.03643
      6   38    4   18    -0.03215         6   38    4   27     0.03164
      8   24    5   29     0.03104         8   35    6   18     0.03059
*******************************************************************************
Singlet       B3G     ***************************************************
###   1-st  ###           ---  13th state in this spin multiplicity ---
    Total energy       in au =     -77.973261
    Correlation energy in au =       0.077611
    Excitation energy  in au =       0.361482    in eV =       9.836418
  *SINGLE EXCITATION
      7    9     0.87340         7   26     0.34181
      7   19    -0.16133         7   16     0.13420
      7   28    -0.06936         7   13     0.06603
  *DOUBLE EXCITATION
      8   27    5    9    -0.12106         8   18    5    9     0.08294
      8   35    7    9     0.06868         8   25    7    9    -0.06726
      8   36    5    9    -0.05993         7   33    7    9    -0.05107
      8   27    5   26    -0.04295         6   38    5    9    -0.03743
      7   29    5    9     0.03552         6   29    4    9     0.03308
      7    9    5   23    -0.03185         7   30    4    9    -0.03169
      7    9    5   34     0.03120
*******************************************************************************
Singlet       AU      ***************************************************
###   1-st  ###           ---   7th state in this spin multiplicity ---
    Total energy       in au =     -78.008032
    Correlation energy in au =       0.042840
    Excitation energy  in au =       0.326711    in eV =       8.890246
```

```
  *SINGLE EXCITATION
       8   12     0.87585         8   22     0.42564
       8   33     0.05030
  *DOUBLE EXCITATION
       8   25    8   12    -0.08725         8   35    8   12     0.08228
       8   12    7   33    -0.07029         8   12    5   29    -0.06478
       8   12    6   32    -0.06220         8   12    4   31     0.06012
       8   12    5   23    -0.05549         8   12    5   34     0.05167
       8   12    7   37     0.04994         8   25    8   22    -0.04006
       8   35    8   22     0.03721         8   12    7   22    -0.03404
       8   12    4   24    -0.03338         8   22    7   33    -0.03273
       8   22    5   29    -0.03211
###   2-nd  ###           ---  18th state in this spin multiplicity ---
    Total energy       in au =     -77.959992
    Correlation energy in au =       0.090880
    Excitation energy  in au =       0.374751    in eV =      10.197482
  *SINGLE EXCITATION
       8   22     0.86699         8   12    -0.42957
       8   33     0.11390         8   37    -0.03914
  *DOUBLE EXCITATION
       8   25    8   22    -0.08281         8   35    8   22     0.07725
       8   22    7   33    -0.06672         8   22    5   29    -0.06452
       8   22    6   32    -0.06027         8   22    4   31     0.05937
       8   22    5   23    -0.05200         8   22    7   37     0.04884
       8   25    8   12     0.04395         8   35    8   12    -0.04164
       8   27    8   23     0.04147         8   22    5   34     0.04040
       8   22    7   22    -0.03511         8   12    7   33     0.03496
       8   22    4   24    -0.03194         8   12    5   29     0.03141
       8   12    6   32     0.03074
*****************************************************************************
Singlet       B1U     ***********************************************************
###   1-st  ###           ---   4th state in this spin multiplicity ---
    Total energy       in au =     -78.033590
    Correlation energy in au =       0.017282
    Excitation energy  in au =       0.301152    in eV =       8.194771
  *SINGLE EXCITATION
       8   18     0.80472         8   14     0.42228
       8   27    -0.34117         6   38     0.06766
       7   29    -0.06281         7   23     0.04848
       4   26     0.04659         6   30    -0.04044
       7   34    -0.03715         5   33     0.03660
  *DOUBLE EXCITATION
       8   36    8   35     0.05423         8   18    5   29    -0.05113
       8   25    8   18    -0.04104         8   25    8   14    -0.03938
       8   35    8   18     0.03832         8   35    8   14     0.03720
       8   18    7   33    -0.03274         8   18    6   32    -0.03185
       8   18    4   31     0.03159         8   14    7   33    -0.03089
       8   14    5   29    -0.03026         8   36    8   25    -0.03012
###   2-nd  ###           ---  11th state in this spin multiplicity ---
```

```
    Total energy       in au =     -77.994951
    Correlation energy in au =       0.055921
    Excitation energy  in au =       0.339791    in eV =       9.246193
  *SINGLE EXCITATION
       8   14     0.85859         8   27     0.35166
       8   18    -0.29195         7   23    -0.04107
       6   38    -0.03922         7   29     0.03210
  *DOUBLE EXCITATION
       8   25    8   14    -0.08953         8   35    8   14     0.08409
       8   14    7   33    -0.07035         8   14    5   29    -0.06349
       8   14    6   32    -0.06216         8   14    4   31     0.05975
       8   14    5   23    -0.05570         8   14    5   34     0.05187
       8   14    7   37     0.04960         8   14    7   22    -0.03389
       8   14    4   24    -0.03356         8   36    8   35    -0.03233
       8   17    8   14    -0.03001
*******************************************************************************
Singlet       B2U     ******************************************************
###   1-st  ###           ---   9th state in this spin multiplicity ---
    Total energy       in au =     -78.006977
    Correlation energy in au =       0.043895
    Excitation energy  in au =       0.327765    in eV =       8.918952
  *SINGLE EXCITATION
       8   15     0.87073         8   20     0.44044
  *DOUBLE EXCITATION
       8   25    8   15    -0.08833         8   35    8   15     0.08321
       8   15    7   33    -0.06987         8   15    5   29    -0.06284
       8   15    6   32    -0.06110         8   15    4   31     0.05881
       8   15    5   23    -0.05517         8   15    5   34     0.05190
       8   15    7   37     0.04854         8   25    8   20    -0.04770
       8   35    8   20     0.04341         8   20    7   33    -0.03455
       8   15    7   22    -0.03329         8   15    4   24    -0.03295
###   2-nd  ###           ---  16th state in this spin multiplicity ---
    Total energy       in au =     -77.962975
    Correlation energy in au =       0.087897
    Excitation energy  in au =       0.371767    in eV =      10.116299
  *SINGLE EXCITATION
       8   20     0.87088         8   15    -0.44037
  *DOUBLE EXCITATION
       8   25    8   20    -0.09379         8   35    8   20     0.08560
       8   20    7   33    -0.06832         8   20    5   29    -0.05928
       8   20    6   32    -0.05894         8   20    4   31     0.05667
       8   20    5   23    -0.05392         8   20    5   34     0.05232
       8   25    8   15     0.04359         8   35    8   15    -0.04171
       8   20    7   37     0.03857         8   15    7   33     0.03546
       8   15    5   29     0.03265         8   20    4   24    -0.03193
       8   15    6   32     0.03146         8   20    7   22    -0.03143
       8   15    4   31    -0.03027
*******************************************************************************
Singlet       B3U     ******************************************************
```

```
###   1-st  ###           ---   1st state in this spin multiplicity ---
    Total energy       in au =     -78.068844
    Correlation energy in au =      -0.017972
    Excitation energy  in au =       0.265899    in eV =       7.235476
  *SINGLE EXCITATION
       8    9     0.87879         8   26     0.34048
       8   16     0.16721         8   19    -0.14907
       8   13     0.07499         8   28    -0.07322
       8   32     0.03968
  *DOUBLE EXCITATION
       8   25    8    9    -0.08920         8   35    8    9     0.08180
       8    9    7   33    -0.06612         8    9    5   29    -0.06218
       8    9    6   32    -0.05927         8    9    4   31     0.05791
       8    9    5   23    -0.05221         8   27    8   24     0.04548
       8    9    5   34     0.04193         8    9    7   37     0.03943
       8   26    8   25    -0.03385         8    9    4   24    -0.03123
       8    9    7   22    -0.03101         8   24    8   18    -0.03083
###   2-nd  ###           ---   6th state in this spin multiplicity ---
    Total energy       in au =     -78.010888
    Correlation energy in au =       0.039984
    Excitation energy  in au =       0.323854    in eV =       8.812525
  *SINGLE EXCITATION
       8   13    -0.75158         8   19    -0.54741
       8   16    -0.26869         8   28    -0.10937
       8   21    -0.06365         8   26     0.03691
       8   32    -0.03339
  *DOUBLE EXCITATION
       8   25    8   13     0.07537         8   35    8   13    -0.07124
       8   13    7   33     0.05919         8   13    5   29     0.05516
       8   13    6   32     0.05408         8   25    8   19     0.05333
       8   13    4   31    -0.05194         8   35    8   19    -0.05072
       8   13    5   23     0.03759         8   13    5   34    -0.03607
       8   13    7   37    -0.03584         8   19    7   33     0.03471
       8   19    4   31    -0.03157         8   19    5   29     0.03155
       8   19    6   32     0.03100
###   3-rd  ###           ---   8th state in this spin multiplicity ---
    Total energy       in au =     -78.007256
    Correlation energy in au =       0.043616
    Excitation energy  in au =       0.327486    in eV =       8.911351
  *SINGLE EXCITATION
       8   16     0.78429         8   21    -0.47198
       8   13    -0.30165         8    9    -0.11932
       8   19     0.08201         8   32    -0.04362
       8   28     0.03027
  *DOUBLE EXCITATION
       8   25    8   16    -0.08189         8   35    8   16     0.07656
       8   16    7   33    -0.06166         8   16    5   29    -0.05572
       8   16    6   32    -0.05498         8   25    8   21     0.05383
       8   16    4   31     0.05243         8   16    5   23    -0.04833
```

```
      8   35    8   21    -0.04790         8   16    5   34     0.03839
      8   16    7   37     0.03603         8   21    7   33     0.03505
      8   21    5   29     0.03258         8   21    6   32     0.03215
      8   21    4   31    -0.03064
###   4-th  ###          ---  12th state in this spin multiplicity ---
    Total energy       in au =     -77.976367
    Correlation energy in au =       0.074505
    Excitation energy  in au =       0.358375    in eV =       9.751888
  *SINGLE EXCITATION
      8   19    -0.66806         8   13     0.46433
      8    9    -0.33022         8   26     0.32185
      8   28    -0.21132         8   16     0.19131
  *DOUBLE EXCITATION
      8   25    8   19     0.06393         8   35    8   19    -0.06119
      8   25    8   13    -0.04698         8   35    8   13     0.04436
      8   19    7   33     0.04159         8   19    4   31    -0.03740
      8   19    5   29     0.03726         8   13    7   33    -0.03694
      8   19    6   32     0.03652         8   25    8    9     0.03589
      8   13    5   29    -0.03342         8   19    5   34    -0.03323
      8   13    6   32    -0.03285         8   35    8    9    -0.03274
      8   19    5   23     0.03201         8   13    4   31     0.03144
###   5-th  ###          ---  15th state in this spin multiplicity ---
    Total energy       in au =     -77.965055
    Correlation energy in au =       0.085817
    Excitation energy  in au =       0.369688    in eV =      10.059719
  *SINGLE EXCITATION
      8   21     0.82380         8   16     0.44374
      8   13    -0.18221         8   26    -0.16421
      8   32     0.09358         8   19    -0.06977
      8   28    -0.05233
  *DOUBLE EXCITATION
      8   25    8   21    -0.09418         8   35    8   21     0.08468
      8   21    7   33    -0.06161         8   21    5   29    -0.05675
      8   21    6   32    -0.05622         8   21    4   31     0.05364
      8   21    5   23    -0.04801         8   25    8   16    -0.04160
      8   35    8   16     0.04081         8   21    5   34     0.03857
      8   21    7   37     0.03633         8   16    7   33    -0.03569
      8   16    5   29    -0.03333         8   16    6   32    -0.03221
      8   16    4   31     0.03097
================================================================
  STEP #DENS#  Density Calculation
================================================================
Transition density for SAC/SAC-CI (V)
Threshold for S2 operators (CThreDensULS2):  0.50D-02
Threshold for R1,R2 operators (CThreDensULR1):  0.10D+00
Only right vectors are used. (ILEFT=0)
--------------------------------------------------------------------------------
Transition dipole moment of   singlet state from SAC ground state
--------------------------------------------------------------------------------
```

```
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
-------------------------------------------------------------------------------
   AG         0      0.0          Excitations are from this state.
   AG         1      8.2227      0.0000      0.0000      0.0000      0.0000
   AG         2     10.5363      0.0000      0.0000      0.0000      0.0000
   B1G        1      7.8776      0.0000      0.0000      0.0000      0.0000
   B1G        2      8.9420      0.0000      0.0000      0.0000      0.0000
   B1G        3      9.9843      0.0000      0.0000      0.0000      0.0000
   B2G        1      7.9015      0.0000      0.0000      0.0000      0.0000
   B2G        2     10.1322      0.0000      0.0000      0.0000      0.0000
   B2G        3     10.3338      0.0000      0.0000      0.0000      0.0000
   B3G        1      9.8364      0.0000      0.0000      0.0000      0.0000
   AU         1      8.8902      0.0000      0.0000      0.0000      0.0000
   AU         2     10.1975      0.0000      0.0000      0.0000      0.0000
   B1U        1      8.1948      0.0000      0.0000     -1.3468      0.3641
   B1U        2      9.2462      0.0000      0.0000      0.5272      0.0630
   B2U        1      8.9190      0.0000     -0.3125      0.0000      0.0213
   B2U        2     10.1163      0.0000     -0.4235      0.0000      0.0445
   B3U        1      7.2355     -0.6789      0.0000      0.0000      0.0817
   B3U        2      8.8125      0.1439      0.0000      0.0000      0.0045
   B3U        3      8.9114     -0.4800      0.0000      0.0000      0.0503
   B3U        4      9.7519     -0.0362      0.0000      0.0000      0.0003
   B3U        5     10.0597      0.6753      0.0000      0.0000      0.1124
-------------------------------------------------------------------------------
================================================================
  STEP #CIMX#  CI matrix elements          ### TRIPLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Triplet   AG    CONVERGED
Solution for Triplet   B1G   CONVERGED
Solution for Triplet   B2G   CONVERGED
Solution for Triplet   B3G   CONVERGED
Solution for Triplet   AU    CONVERGED
Solution for Triplet   B1U   CONVERGED
Solution for Triplet   B2U   CONVERGED
Solution for Triplet   B3U   CONVERGED
================================================================
  STEP #ULINTT#  Unlinked integral for Triplet State (SAC-CI)
================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
================================================================
  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
================================================================
```

```
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Triplet   AG    CONVERGED
Solution for Triplet   B1G   CONVERGED
Solution for Triplet   B2G   CONVERGED
Solution for Triplet   B3G   CONVERGED
Solution for Triplet   AU    CONVERGED
Solution for Triplet   B1U   CONVERGED
Solution for Triplet   B2U   CONVERGED
Solution for Triplet   B3U   CONVERGED
***********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
***********************************************
*******************************************************************************
Triplet       AG      ******************************************************
###   1-st  ###           ---   5th state in this spin multiplicity ---
    Total energy       in au =     -78.038528
    Correlation energy in au =       0.012344
    Excitation energy  in au =       0.296214    in eV =       8.060406
  *SINGLE EXCITATION
       8   17    -0.88401         8   25    -0.41192
       8   35     0.06955
  *DOUBLE EXCITATION
       8   35    8   17    -0.08426         8   25    8   17     0.07457
       7   33    8   17     0.06974         5   29    8   17     0.06316
       6   32    8   17     0.06155         4   31    8   17    -0.05921
       5   23    8   17     0.05462         5   34    8   17    -0.05097
       7   37    8   17    -0.04803         8   35    8   25    -0.03802
       4   24    8   17     0.03249         7   22    8   17     0.03188
###   2-nd  ###           ---  20th state in this spin multiplicity ---
    Total energy       in au =     -77.956953
    Correlation energy in au =       0.093919
    Excitation energy  in au =       0.377790    in eV =      10.280180
  *SINGLE EXCITATION
       8   25    -0.87676         8   17     0.41335
       8   35     0.13798
  *DOUBLE EXCITATION
       8   35    8   25    -0.07830         8   25    8   17    -0.07743
       7   33    8   25     0.06105         6   32    8   25     0.05598
       5   29    8   25     0.05533         4   31    8   25    -0.05339
       8   35    8   17     0.04254         5   34    8   25    -0.03854
       5   25    8   23    -0.03727         8   25    5   23    -0.03702
       7   33    8   17    -0.03634         7   37    8   25    -0.03440
       8   23    5   25    -0.03325         5   29    8   17    -0.03313
       6   32    8   17    -0.03183         4   31    8   17     0.03048
*******************************************************************************
Triplet       B1G     ******************************************************
###   1-st  ###           ---   4th state in this spin multiplicity ---
    Total energy       in au =     -78.046505
```

```
    Correlation energy in au =       0.004367
    Excitation energy  in au =       0.288237    in eV =       7.843337
  *SINGLE EXCITATION
       8   11     0.84336         8   23     0.47365
       8   29     0.09890         8   34    -0.07824
       7   27     0.04246         7   18    -0.03751
  *DOUBLE EXCITATION
       8   25    8   11    -0.08161         8   35    8   11     0.07772
       7   33    8   11    -0.06672         5   29    8   11    -0.06044
       6   32    8   11    -0.05827         4   31    8   11     0.05726
       5   23    8   11    -0.04458         5   34    8   11     0.04206
       7   37    8   11     0.03933         8   25    8   23    -0.03900
       8   35    8   23     0.03809         7   33    8   23    -0.03199
       4   24    8   11    -0.03075
###   2-nd  ###           ---   6th state in this spin multiplicity ---
    Total energy       in au =     -78.018776
    Correlation energy in au =       0.032096
    Excitation energy  in au =       0.315966    in eV =       8.597878
  *SINGLE EXCITATION
       7   18     0.70681         7   27    -0.63909
       7   14     0.13467         7   36    -0.12087
       8   11     0.07205
  *DOUBLE EXCITATION
       8   27    5   18    -0.10726         8   27    5   27     0.09048
       8   18    5   27    -0.07396         8   18    5   18     0.07245
       8   36    5   18    -0.03770         8   35    7   36     0.03575
       6   38    5   18    -0.03252
###   3-rd  ###           ---  15th state in this spin multiplicity ---
    Total energy       in au =     -77.970022
    Correlation energy in au =       0.080850
    Excitation energy  in au =       0.364720    in eV =       9.924545
  *SINGLE EXCITATION
       8   23     0.81100         8   11    -0.48582
       8   29     0.21049         8   34    -0.12999
       7   18     0.04028
  *DOUBLE EXCITATION
       8   25    8   23    -0.07092         8   35    8   23     0.06807
       7   33    8   23    -0.05608         8   25    8   11     0.05248
       8   35    8   11    -0.04911         5   23    8   11     0.04785
       7   33    8   11     0.04184         4   31    8   23     0.04164
       5   29    8   23    -0.03991         5   29    8   11     0.03923
       6   32    8   11     0.03855         6   32    8   23    -0.03788
       5   34    8   23     0.03751         4   31    8   11    -0.03556
       7   37    8   23     0.03447         8   33    8   27    -0.03205
       8   23    5   23     0.03067
*******************************************************************************
Triplet       B2G     ******************************************************
###   1-st  ###           ---   3rd state in this spin multiplicity ---
    Total energy       in au =     -78.046654
```

```
    Correlation energy in au =       0.004218
    Excitation energy  in au =       0.288088    in eV =       7.839276
  *SINGLE EXCITATION
       8   10     0.86151         8   24     0.43761
       8   31    -0.12222
  *DOUBLE EXCITATION
       8   25    8   10    -0.08318         8   35    8   10     0.07924
       7   33    8   10    -0.06779         5   29    8   10    -0.06646
       6   32    8   10    -0.06214         4   31    8   10     0.06021
       5   23    8   10    -0.05239         7   37    8   10     0.04996
       5   34    8   10     0.04097         8   27    8    9     0.04017
       8   27    8   26     0.03997         8   25    8   24    -0.03670
       8   35    8   24     0.03613         5   29    8   24    -0.03289
       7   22    8   10    -0.03046
###   2-nd  ###           ---  13th state in this spin multiplicity ---
    Total energy       in au =     -77.978033
    Correlation energy in au =       0.072839
    Excitation energy  in au =       0.356709    in eV =       9.706551
  *SINGLE EXCITATION
       6   18     0.67722         6   27    -0.66810
       6   36    -0.15921         6   14     0.11675
       8   24     0.05011         3   27     0.04761
       8   10    -0.04635         8   30     0.03035
  *DOUBLE EXCITATION
       8   27    4   18    -0.07532         8   27    4   27     0.06790
       8   18    4   27    -0.05480         8   18    4   18     0.05238
       8   35    6   18     0.03314         8   36    6   35     0.03252
       8   35    6   36     0.03200
###   3-rd  ###           ---  18th state in this spin multiplicity ---
    Total energy       in au =     -77.963965
    Correlation energy in au =       0.086907
    Excitation energy  in au =       0.370777    in eV =      10.089361
  *SINGLE EXCITATION
       8   24     0.82924         8   10    -0.45439
       8   31    -0.21917         6   27     0.04974
       8   40     0.04756         6   18    -0.04494
       8   30    -0.04118
  *DOUBLE EXCITATION
       8   25    8   24    -0.07444         8   35    8   24     0.07215
       5   29    8   24    -0.06038         8   27    8   26     0.05577
       7   33    8   24    -0.05537         6   32    8   24    -0.05430
       8   25    8   10     0.04897         8   35    8   10    -0.04548
       4   31    8   24     0.04363         7   33    8   10     0.04033
       8   24    5   23     0.03743         7   37    8   24     0.03678
       6   32    8   10     0.03580         5   34    8   24     0.03551
       5   24    8   23     0.03494         5   29    8   10     0.03439
       4   31    8   10    -0.03420         8   23    5   24     0.03290
       5   23    8   10     0.03186
*******************************************************************************
```

```
Triplet       B3G     ********************************************************
###   1-st  ###           ---  12th state in this spin multiplicity ---
    Total energy       in au =     -77.980852
    Correlation energy in au =       0.070020
    Excitation energy  in au =       0.353891    in eV =       9.629860
  *SINGLE EXCITATION
       7    9     0.83686         7   26     0.38634
       7   19    -0.18676         7   16     0.12550
       7   28    -0.11301         5   24     0.08980
       5   10     0.06449         7   13     0.06410
       7   32     0.05722         4   23     0.05259
       7   39     0.03417
  *DOUBLE EXCITATION
       8   27    5    9    -0.12687         8   18    5    9     0.08664
       8   35    7    9     0.07067         8   25    7    9    -0.07011
       8   36    5    9    -0.06291         8   27    5   26    -0.04999
       7   33    7    9    -0.03875         6   38    5    9    -0.03540
       7   29    5    9     0.03238         5   27    8    9    -0.03212
       6   29    4    9     0.03129
*************************************************************************
Triplet       AU      ********************************************************
###   1-st  ###           ---   8th state in this spin multiplicity ---
    Total energy       in au =     -78.008256
    Correlation energy in au =       0.042616
    Excitation energy  in au =       0.326487    in eV =       8.884155
  *SINGLE EXCITATION
       8   12     0.87266         8   22     0.43167
       8   33     0.05402
  *DOUBLE EXCITATION
       8   25    8   12    -0.08684         8   35    8   12     0.08202
       7   33    8   12    -0.07159         5   29    8   12    -0.06595
       6   32    8   12    -0.06324         4   31    8   12     0.06099
       5   23    8   12    -0.05649         5   34    8   12     0.05278
       7   37    8   12     0.05092         8   25    8   22    -0.04036
       8   35    8   22     0.03809         7   33    8   22    -0.03445
       5   29    8   22    -0.03337         4   24    8   12    -0.03333
       7   22    8   12    -0.03109         4   31    8   22     0.03061
       6   32    8   22    -0.03002
###   2-nd  ###           ---  19th state in this spin multiplicity ---
    Total energy       in au =     -77.960554
    Correlation energy in au =       0.090318
    Excitation energy  in au =       0.374189    in eV =      10.182191
  *SINGLE EXCITATION
       8   22     0.86330         8   12    -0.43591
       8   33     0.11870         8   37    -0.04312
  *DOUBLE EXCITATION
       8   25    8   22    -0.08195         8   35    8   22     0.07750
       7   33    8   22    -0.06766         5   29    8   22    -0.06591
       4   31    8   22     0.06059         6   32    8   22    -0.05984
```

```
      5   23    8   22    -0.05262         7   37    8   22     0.05072
      8   25    8   12     0.04468         5   34    8   22     0.04265
      8   35    8   12    -0.04214         8   27    8   23     0.03819
      7   33    8   12     0.03618         5   29    8   12     0.03242
      6   32    8   12     0.03182         4   24    8   22    -0.03077
      4   31    8   12    -0.03018
*****************************************************************************
Triplet       B1U     ******************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    Total energy       in au =     -78.168725
    Correlation energy in au =      -0.117853
    Excitation energy  in au =       0.166018    in eV =       4.517575
  *SINGLE EXCITATION
      8   27     0.70065         8   18    -0.66390
      8   36     0.17461         8   14    -0.11012
  *DOUBLE EXCITATION
      8   35    8   18    -0.03849         8   31    4   27     0.03657
      8   35    8   27     0.03377         8   25    8   18     0.03336
###   2-nd  ###           ---  11th state in this spin multiplicity ---
    Total energy       in au =     -78.003102
    Correlation energy in au =       0.047770
    Excitation energy  in au =       0.331640    in eV =       9.024390
  *SINGLE EXCITATION
      8   14     0.92620         8   27     0.26866
      8   18     0.14161         8   36     0.05113
  *DOUBLE EXCITATION
      8   25    8   14    -0.09287         8   35    8   14     0.08816
      7   33    8   14    -0.07602         5   29    8   14    -0.06971
      6   32    8   14    -0.06623         4   31    8   14     0.06446
      5   23    8   14    -0.05976         5   34    8   14     0.05503
      7   37    8   14     0.05361         7   22    8   14    -0.03576
      4   24    8   14    -0.03530
*****************************************************************************
Triplet       B2U     ******************************************************
###   1-st  ###           ---   9th state in this spin multiplicity ---
    Total energy       in au =     -78.007575
    Correlation energy in au =       0.043297
    Excitation energy  in au =       0.327168    in eV =       8.902684
  *SINGLE EXCITATION
      8   15     0.85936         8   20     0.46261
  *DOUBLE EXCITATION
      8   25    8   15    -0.08667         8   35    8   15     0.08209
      7   33    8   15    -0.07026         5   29    8   15    -0.06333
      6   32    8   15    -0.06149         4   31    8   15     0.05898
      5   23    8   15    -0.05535         5   34    8   15     0.05126
      7   37    8   15     0.04893         8   35    8   20     0.04427
      8   25    8   20    -0.04390         7   33    8   20    -0.03677
      7   22    8   15    -0.03284         4   24    8   15    -0.03259
      5   29    8   20    -0.03255         6   32    8   20    -0.03164
```

```
      4   31    8   20     0.03034
###   2-nd  ###          ---  17th state in this spin multiplicity ---
    Total energy       in au =     -77.964863
    Correlation energy in au =       0.086009
    Excitation energy  in au =       0.369879    in eV =      10.064924
  *SINGLE EXCITATION
      8   20     0.85997         8   15    -0.46215
  *DOUBLE EXCITATION
      8   35    8   20     0.08170         8   25    8   20    -0.08117
      7   33    8   20    -0.06841         5   29    8   20    -0.06154
      6   32    8   20    -0.05960         4   31    8   20     0.05710
      5   34    8   20     0.05209         5   23    8   20    -0.05147
      7   37    8   20     0.04753         8   25    8   15     0.04715
      8   35    8   15    -0.04388         7   33    8   15     0.03797
      5   29    8   15     0.03480         6   32    8   15     0.03361
      4   31    8   15    -0.03224         4   24    8   20    -0.03108
      7   22    8   20    -0.03052         5   23    8   15     0.03017
*****************************************************************************
Triplet       B3U     ******************************************************
###   1-st  ###          ---   2nd state in this spin multiplicity ---
    Total energy       in au =     -78.072975
    Correlation energy in au =      -0.022103
    Excitation energy  in au =       0.261768    in eV =       7.123062
  *SINGLE EXCITATION
      8    9     0.85767         8   26     0.39103
      8   16     0.16926         8   19    -0.15389
      8   28    -0.07694         8   13     0.06798
      8   21    -0.04743         8   39     0.03358
  *DOUBLE EXCITATION
      8   25    8    9    -0.07812         8   35    8    9     0.07791
      7   33    8    9    -0.06460         5   29    8    9    -0.06159
      6   32    8    9    -0.05981         4   31    8    9     0.05845
      8   27    8   24     0.04047         5   34    8    9     0.03960
      7   37    8    9     0.03882         5   23    8    9    -0.03743
      4   24    8    9    -0.03114
###   2-nd  ###          ---   7th state in this spin multiplicity ---
    Total energy       in au =     -78.010028
    Correlation energy in au =       0.040844
    Excitation energy  in au =       0.324714    in eV =       8.835917
  *SINGLE EXCITATION
      8   13     0.65238         8   19     0.59274
      8   16     0.39504         8   28     0.14373
      8   21    -0.06315
  *DOUBLE EXCITATION
      8   25    8   13    -0.06565         8   35    8   13     0.06233
      8   25    8   19    -0.05605         8   35    8   19     0.05461
      7   33    8   13    -0.05204         8   25    8   16    -0.04049
      5   29    8   13    -0.03900         8   35    8   16     0.03892
      6   32    8   13    -0.03790         4   31    8   13     0.03773
```

```
      7   33    8   19    -0.03590         5   29    8   19    -0.03430
      4   31    8   19     0.03315         6   32    8   19    -0.03282
      5   23    8   13    -0.03233         7   33    8   16    -0.03143
      5   34    8   13     0.03140         7   37    8   13     0.03084
###   3-rd  ###           ---  10th state in this spin multiplicity ---
    Total energy       in au =     -78.007237
    Correlation energy in au =       0.043635
    Excitation energy  in au =       0.327505    in eV =       8.911872
  *SINGLE EXCITATION
      8   16    -0.65574         8   21     0.54589
      8   13     0.43541         8    9     0.15854
      8   32     0.08624         8   26    -0.08579
      8   28    -0.03327
  *DOUBLE EXCITATION
      8   25    8   16     0.06638         8   35    8   16    -0.06396
      7   33    8   16     0.05202         8   35    8   21     0.05045
      8   25    8   21    -0.04835         8   25    8   13    -0.04383
      8   35    8   13     0.04131         7   33    8   21    -0.04081
      5   29    8   16     0.03761         6   32    8   16     0.03720
      4   31    8   16    -0.03676         7   33    8   13    -0.03468
      5   23    8   16     0.03203         5   34    8   16    -0.03162
      5   29    8   21    -0.03024
###   4-th  ###           ---  14th state in this spin multiplicity ---
    Total energy       in au =     -77.977753
    Correlation energy in au =       0.073119
    Excitation energy  in au =       0.356989    in eV =       9.714175
  *SINGLE EXCITATION
      8   19    -0.58575         8   13     0.50680
      8   26     0.39330         8    9    -0.37046
      8   28    -0.20895         8   16     0.13086
      8   21    -0.06722         8   39     0.03126
  *DOUBLE EXCITATION
      8   25    8   19     0.05489         8   35    8   19    -0.05369
      8   25    8   13    -0.05173         8   35    8   13     0.04888
      8   25    8    9     0.04224         7   33    8   13    -0.04106
      8   35    8    9    -0.03901         5   29    8   19     0.03359
      7   33    8   19     0.03344         7   33    8    9     0.03310
      4   31    8   19    -0.03224         6   32    8   19     0.03203
###   5-th  ###           ---  16th state in this spin multiplicity ---
    Total energy       in au =     -77.969768
    Correlation energy in au =       0.081104
    Excitation energy  in au =       0.364975    in eV =       9.931472
  *SINGLE EXCITATION
      8   21     0.69946         8   16     0.57048
      8   26    -0.27231         8   19    -0.18823
      8   32     0.12023         8   28    -0.11169
      8   13    -0.09594
  *DOUBLE EXCITATION
      8   35    8   21     0.06356         8   25    8   16    -0.06125
```

```
      8   25    8   21    -0.05966        8   35    8   16     0.05580
      7   33    8   21    -0.05237        7   33    8   16    -0.04613
      5   29    8   21    -0.03783        6   32    8   21    -0.03753
      4   31    8   21     0.03745        5   29    8   16    -0.03397
      4   31    8   16     0.03329        6   32    8   16    -0.03314
      5   34    8   21     0.03256        5   23    8   21    -0.03181
================================================================
  STEP #DENS#  Density Calculation
================================================================
Transition density for SAC/SAC-CI (V)
Threshold for S2 operators (CThreDensULS2):  0.50D-02
Threshold for R1,R2 operators (CThreDensULR1):  0.10D+00
Left and right vectors are used. (ILEFT=1)
--------------------------------------------------------------------------------
Transition dipole moment of   triplet state from symmetry B1U    1-th state
--------------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
--------------------------------------------------------------------------------
   AG         1      3.5428      0.0000      0.0000     -0.4580      0.0182
   AG         2      5.7626      0.0000      0.0000     -0.2063      0.0060
   B1G        1      3.3258      0.0000      0.0000      0.0000      0.0000
   B1G        2      4.0803      0.0000      0.0000      0.0000      0.0000
   B1G        3      5.4070      0.0000      0.0000      0.0000      0.0000
   B2G        1      3.3217      0.5663      0.0000      0.0000      0.0261
   B2G        2      5.1890     -0.1117      0.0000      0.0000      0.0016
   B2G        3      5.5718      0.3176      0.0000      0.0000      0.0138
   B3G        1      5.1123      0.0000     -0.0208      0.0000      0.0001
   AU         1      4.3666      0.0000      0.0000      0.0000      0.0000
   AU         2      5.6646      0.0000      0.0000      0.0000      0.0000
   B1U        1      0.0          Excitations are from this state.
   B1U        2      4.5068      0.0000      0.0000      0.0000      0.0000
   B2U        1      4.3851      0.0000      0.0000      0.0000      0.0000
   B2U        2      5.5473      0.0000      0.0000      0.0000      0.0000
   B3U        1      2.6055      0.0000      0.0000      0.0000      0.0000
   B3U        2      4.3183      0.0000      0.0000      0.0000      0.0000
   B3U        3      4.3943      0.0000      0.0000      0.0000      0.0000
   B3U        4      5.1966      0.0000      0.0000      0.0000      0.0000
   B3U        5      5.4139      0.0000      0.0000      0.0000      0.0000
--------------------------------------------------------------------------------
================================================================
  STEP #CIMX#  CI matrix elements          ### IONIZED STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Ionized   AG    CONVERGED
```

```
Solution for Ionized   B3G   CONVERGED
Solution for Ionized   B1U   CONVERGED
Solution for Ionized   B2U   CONVERGED
Solution for Ionized   B3U   CONVERGED
================================================================
  STEP #ULINTIA#  Unlinked integral for Ionized State (SAC-CI)
================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
================================================================
  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Ionized   AG    CONVERGED
Solution for Ionized   B3G   CONVERGED
Solution for Ionized   B1U   CONVERGED
Solution for Ionized   B2U   CONVERGED
Solution for Ionized   B3U   CONVERGED
**********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
**********************************************
*****************************************************************************
CationDoublet AG      ******************************************************
###   1-st  ###           ---   3rd state in this spin multiplicity ---
    Total energy       in au =     -77.795397
    Correlation energy in au =       0.255475
    Excitation energy  in au =       0.539346    in eV =      14.676347
  *SINGLE EXCITATION
       6     0.96084
  *DOUBLE EXCITATION
       8   35    6     0.10618         8   27    4    -0.09855
       8   25    6    -0.09408         7   33    6    -0.07745
       6   32    6    -0.07519         8   18    4     0.06832
       5   34    6     0.06524         5   23    6    -0.05981
       5   29    6    -0.04690         8   36    4    -0.04533
       6   38    4    -0.04093         7   29    4     0.04010
       4   31    6     0.03924         7   28    7    -0.03771
       4   24    6    -0.03679         5   29    3     0.03619
       8   45    3     0.03554         7   22    6    -0.03537
       3   39    6    -0.03331         6   26    6    -0.03243
       6   32    3     0.03033
###   2-nd  ###           ---   6th state in this spin multiplicity ---
    Total energy       in au =     -77.439540
    Correlation energy in au =       0.611332
    Excitation energy  in au =       0.895203    in eV =      24.359704
  *SINGLE EXCITATION
       3     0.85466
  *DOUBLE EXCITATION
```

```
      8   27    4    -0.30224         4   27    8    -0.25020
      8   18    4     0.21453         8   28    8     0.19027
      4   18    8     0.17720         8   32    8    -0.13634
      8   36    4    -0.13597         8   35    3     0.11309
      4   36    8    -0.11046         8   19    8     0.09793
      8   25    3    -0.09607         8    9    8    -0.09223
      8   26    8    -0.08679         8   21    8    -0.08315
      5   29    6     0.08025         6   29    5     0.07798
      7   33    3    -0.07723         5   29    3    -0.07481
      7   28    7    -0.07331         8   45    6     0.07325
      6   32    3    -0.07263         7   30    5    -0.07051
      4   31    3     0.06722         5   34    3     0.06147
      6   32    6     0.06058         5   23    3    -0.05914
      6   45    8     0.05834         8   44    5     0.05583
      8   42    8     0.05144         5   28    5    -0.05032
      8   50    8     0.04900         6   38    4    -0.04384
      6   41    5    -0.04244         7   37    3     0.04213
      5   41    6    -0.04109         5   30    7    -0.03956
      8   47    7     0.03954         5   44    8     0.03906
      7   42    7    -0.03754         7   37    6    -0.03687
      4   38    6    -0.03677         7   33    6     0.03563
      7   43    5     0.03510         4   24    3    -0.03485
      4   40    3    -0.03483         3   35    8     0.03386
      7   47    8     0.03364         5   23    6     0.03329
      7   22    3    -0.03294         5   34    6    -0.03187
*****************************************************************************
CationDoublet B3G     ****************************************************
###   1-st  ###           ---   2nd state in this spin multiplicity ---
    Total energy       in au =     -77.856703
    Correlation energy in au =       0.194169
    Excitation energy  in au =       0.478040    in eV =      13.008120
  *SINGLE EXCITATION
      7     0.96569
  *DOUBLE EXCITATION
      8   27    5    -0.13719         8   18    5     0.09427
      8   25    7    -0.08027         8   35    7     0.07966
      8   36    5    -0.06843         7   33    7    -0.05797
      7   29    5     0.05120         6   38    5    -0.04160
      5   23    7    -0.03695         6   29    4     0.03653
      5   34    7     0.03510         7   30    4    -0.03495
      7   41    5    -0.03344         7   22    7    -0.03290
      7   43    4     0.03253         8   44    4     0.03158
      5   27    8    -0.03117
*****************************************************************************
CationDoublet B1U     ****************************************************
###   1-st  ###           ---   5th state in this spin multiplicity ---
    Total energy       in au =     -77.618112
    Correlation energy in au =       0.432760
    Excitation energy  in au =       0.716630    in eV =      19.500499
```

```
  *SINGLE EXCITATION
       4     0.92341
  *DOUBLE EXCITATION
       8   27    6    -0.22472         8   18    6     0.16354
       8   27    3    -0.12307         8   35    4     0.09133
       6   27    8    -0.09084         8   36    6    -0.09028
       8   25    4    -0.08515         8   18    3     0.08440
       7   30    7    -0.08358         8   31    8     0.07777
       6   29    7     0.07771         7   29    6     0.07520
       6   18    8     0.06620         8   36    3    -0.06398
       5   28    7    -0.06233         7   33    4    -0.06144
       3   27    8    -0.06120         6   38    6    -0.05905
       7   43    7     0.05460         7   28    5    -0.04832
       6   41    7    -0.04125         5   34    4     0.03944
       8   45    4     0.03842         3   18    8     0.03833
       5   42    7    -0.03789         6   38    3    -0.03788
       7   42    5    -0.03780         7   41    6    -0.03771
       6   26    4    -0.03657         5   23    4    -0.03654
       4   24    4    -0.03542         6   32    4    -0.03352
       4   31    4     0.03293         4   38    4    -0.03252
       6   36    8    -0.03140         3   36    8    -0.03138
       8   47    5     0.03127         8   44    7     0.03124
       8   38    8     0.03122         7   22    4    -0.03109
*******************************************************************************
CationDoublet B2U     ******************************************************
###   1-st  ###           ---   4th state in this spin multiplicity ---
    Total energy       in au =     -77.740282
    Correlation energy in au =       0.310590
    Excitation energy  in au =       0.594460    in eV =      16.176091
  *SINGLE EXCITATION
       5     0.94141
  *DOUBLE EXCITATION
       8   27    7    -0.22746         8   18    7     0.16320
       8   36    7    -0.10009         8   35    5     0.08914
       8   25    5    -0.08710         7   27    8    -0.07191
       7   33    5    -0.06455         7   29    7     0.06417
       5   23    5    -0.05197         7   18    8     0.05118
       6   38    7    -0.04215         5   29    5    -0.03987
       5   34    5     0.03892         7   41    7    -0.03682
       6   32    5    -0.03568         7   22    5    -0.03423
       4   31    5     0.03316         8   44    3     0.03215
       7   36    8    -0.03069         4   24    5    -0.03052
*******************************************************************************
CationDoublet B3U     ******************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    Total energy       in au =     -77.953627
    Correlation energy in au =       0.097245
    Excitation energy  in au =       0.381115    in eV =      10.370668
  *SINGLE EXCITATION
```

```
      8     0.97533
  *DOUBLE EXCITATION
      8   25    8    -0.09810        8   35    8     0.09265
      7   33    8    -0.07895        5   29    8    -0.07149
      6   32    8    -0.06909        4   31    8     0.06653
      5   23    8    -0.06194        5   34    8     0.05786
      7   37    8     0.05537        7   22    8    -0.04751
      4   24    8    -0.03722        8   17    8    -0.03164
================================================================
  STEP #SATEI#  Monopole Intensity Calculation
================================================================
Symmetry  State     I.P.        Intensity
-----------------------------------------
AG          1      14.676       0.92341
            2      24.360       0.73044
-----------------------------------------
B3G         1      13.008       0.93255
-----------------------------------------
B1U         1      19.500       0.85269
-----------------------------------------
B2U         1      16.176       0.88626
-----------------------------------------
B3U         1      10.371       0.95127
-----------------------------------------
================================================================
  STEP #DENS#  Density Calculation
================================================================
Transition density for SAC/SAC-CI (V)
Threshold for S2 operators (CThreDensULS2):  0.50D-02
Threshold for R1,R2 operators (CThreDensULR1):  0.10D+00
Left and right vectors are used. (ILEFT=1)
--------------------------------------------------------------------------------
Transition dipole moment of   ionized state from symmetry B3U    1-th state
--------------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
--------------------------------------------------------------------------------
   AG         1      4.3057      0.1141      0.0000      0.0000      0.0014
   AG         2     13.9890      0.3967      0.0000      0.0000      0.0539
   B3G        1      2.6375      0.0000      0.0000      0.0000      0.0000
   B1U        1      9.1298      0.0000      0.0000      0.0000      0.0000
   B2U        1      5.8054      0.0000      0.0000      0.0000      0.0000
   B3U        1      0.0          Excitations are from this state.
--------------------------------------------------------------------------------
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.

*********************************************************************
```

```
          Population analysis using the SCF density.

**********************************************************************

Orbital symmetries:
      Occupied  (AG) (B1U) (AG) (B1U) (B2U) (AG) (B3G) (B3U)
      Virtual   (AG) (B1U) (B2U) (B3G) (AG) (B2G) (B1G) (AG) (B3U)
                (B2G) (AG) (B1G) (AG) (B3G) (B2U) (B1U) (B3U)
                (AG) (B2G) (AG) (B2U) (B1U) (B1U) (AG) (B3G) (B2U)
                (B3U) (B2G) (B3G) (B1U) (AG) (B1U) (B2U) (AG)
                (B1U) (B1G) (B3U) (B3G) (AU) (AG) (B3G) (AG) (B2U)
                (B1U) (B2G) (B2U) (B3U) (B1G) (B1U) (B2G) (AU)
                (AG) (B3G) (B1U) (AG) (B2U) (B1U) (B3G) (AG) (B1U)
The electronic state is 1-AG.
Alpha  occ. eigenvalues --  -11.24168 -11.24006  -1.03312  -0.79239  -0.64303
Alpha  occ. eigenvalues --   -0.58530  -0.50819  -0.37482
Alpha virt. eigenvalues --    0.03169   0.03468   0.03508   0.03551   0.03554
Alpha virt. eigenvalues --    0.03594   0.03658   0.03681   0.03845   0.10243
Alpha virt. eigenvalues --    0.11738   0.12373   0.12463   0.12670   0.15159
Alpha virt. eigenvalues --    0.15506   0.16761   0.18701   0.19263   0.36642
Alpha virt. eigenvalues --    0.36675   0.39651   0.42002   0.50170   0.56519
Alpha virt. eigenvalues --    0.63239   0.67847   0.68330   0.69338   0.87168
Alpha virt. eigenvalues --    0.96023   1.13895   1.20076   1.32574   1.33696
Alpha virt. eigenvalues --    1.53533   1.56517   1.60212   1.67370   1.96825
Alpha virt. eigenvalues --    2.07478   2.10752   2.11875   2.22033   2.24784
Alpha virt. eigenvalues --    2.43427   2.48609   2.56965   2.61687   2.78096
Alpha virt. eigenvalues --    2.84691   2.94824   2.99706   3.21255   3.36390
Alpha virt. eigenvalues --    3.51834   3.70422   3.93431  24.04900  24.38610
         Condensed to atoms (all electrons):
              1          2          3          4          5          6
    1  H    0.527370   0.412861  -0.038682  -0.005602   0.002285  -0.030002
    2  C    0.412861   4.861946   0.619506  -0.038682  -0.038682   0.412861
    3  C   -0.038682   0.619506   4.861946   0.412861   0.412861  -0.038682
    4  H   -0.005602  -0.038682   0.412861   0.527370  -0.030002   0.002285
    5  H    0.002285  -0.038682   0.412861  -0.030002   0.527370  -0.005602
    6  H   -0.030002   0.412861  -0.038682   0.002285  -0.005602   0.527370
    7  Bq   0.006713   0.002089   0.002089   0.006713   0.006713   0.006713
              7
    1  H    0.006713
    2  C    0.002089
    3  C    0.002089
    4  H    0.006713
    5  H    0.006713
    6  H    0.006713
    7  Bq   0.005399
Mulliken atomic charges:
              1
    1  H    0.125057
    2  C   -0.231900
```

```
    3  C   -0.231900
    4  H    0.125057
    5  H    0.125057
    6  H    0.125057
    7  Bq  -0.036428
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  H    0.000000
    2  C    0.018214
    3  C    0.018214
    4  H    0.000000
    5  H    0.000000
    6  H    0.000000
    7  Bq  -0.036428
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    83.5302
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     0.0000    Y=     0.0000    Z=     0.0000  Tot=     0.0000
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=   -16.2640   YY=   -12.2863   ZZ=   -12.1376
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -2.7013   YY=     1.2763   ZZ=     1.4250
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=     0.0000  YYY=     0.0000  ZZZ=     0.0000  XYY=     0.0000
 XXY=     0.0000  XXZ=     0.0000  XZZ=     0.0000  YZZ=     0.0000
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=   -21.6535 YYYY=   -27.0739 ZZZZ=   -68.5119 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=    -8.8502 XXZZ=   -16.1757 YYZZ=   -13.1232
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 3.324999423628D+01 E-N=-2.476162242765D+02  KE= 7.785168423628D+01
Symmetry AG   KE= 3.748532068494D+01
Symmetry B1G  KE= 9.684633491136D-34
Symmetry B2G  KE= 3.251299784892D-32
Symmetry B3G  KE= 2.083198795373D+00
Symmetry AU   KE= 1.257391018236D-33
Symmetry B1U  KE= 3.454340302188D+01
Symmetry B2U  KE= 1.827961283940D+00
Symmetry B3U  KE= 1.911800450144D+00

Test job not archived.
1¥1¥GINC-MIRAI86¥SP¥RSACCI¥Gen¥C2H4N1¥MASAHIRO¥31-Jul-2004¥0¥¥# SAC-CI
(LEVELTHREE, SINGLET=(NSTATE=(2,3,3,1,2,2,2,5)), TRIPLET=(NSTATE=(2,3,
3,1,2,2,2,5)), CATIONDOUBLET=(NSTATE=(2,0,0,1,0,1,1,1))) /GEN MASSAGE
```

```
SYMM=ON TEST¥¥Gaussian Test Job 635 (Part 3): SAC-CI SD-R LevelThree c
alculations for ethylene¥¥0,1¥H¥C,1,1.0868¥C,2,1.3391,1,121.28¥H,3,1.0
868,2,121.28,1,0.,0¥H,3,1.0868,2,121.28,1,180.,0¥H,2,1.0868,3,121.28,4
,180.,0¥Bq,2,0.66955,1,121.28,4,0.,0¥¥Version=AI64T-G03RevC.02¥State=1
-AG¥HF=-78.050872¥RMSD=3.635e-09¥PG=D02H [O(N1),C2"(C1.C1),SG(H4)]¥¥@


THOSE WHO TRY TO PASS CHEMISTRY OFF AS A NEW SCIENCE
SHOW HOW LITTLE KNOWLEDGE THEY HAVE OF THE CHARACTER
AND LITERATURE OF THE ANCIENTS.
  -- NICOLAS LEFEVRE
"COURS DE CHYMIE" J.-N.LELOUP, PARIS, 1751
Job cpu time:  0 days  0 hours  9 minutes  2.9 seconds.
File lengths (MBytes):  RWF=    678 Int=      0 D2E=      0 Chk=     16 Scr=     48
Normal termination of Gaussian 03 at Sat Jul 31 12:07:45 2004.
```

Output 637

```
Entering Gaussian System, Link 0=/work/g03.C02/g03/g03
Initial command:
/work/g03.C02/g03/l1.exe /work/g03.C02/inputs/Gau-113664.inp -scrdir=/work/g03.C02/inputs/
Entering Link 1 = /work/g03.C02/g03/l1.exe PID=    113667.

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This is the Gaussian(R) 03 program.  It is based on the
the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),
the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),
the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),
the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),
the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),
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Cite this work as:
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M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
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A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

****
Gaussian 03: AI64T-G03RevC.02 12-Jun-2004
31-Jul-2004
****

List of keywords given in the Gaussian input

```
%mem=700MB
-----------------------------------------------------------------------
# SAC-CI(Singlet=(NState=(0,0,0,0,0,4,4,1)), LevelOne,Window=(25,244))
/Gen Test
-----------------------------------------------------------------------
1/38=1/1;
2/17=6,18=5,40=1/2;
3/5=7,11=9,16=1,25=1,30=1,36=2/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=5,9=30000,10=91,37=25,38=244,40=1,42=2/1,4;
9//23;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;
-----------------------------------------------------------------------
Gaussian Test Job 637: SAC-CI SD-R LevelOne calculation of optically-a
llowed singlet excited states of Free-Base Porphin using Huzinaga basi
s sets [4s2p/2s]. Inner-shells are excluded from the active space and
full-valence active MOs are used (FC; default): 57 occupied and 163 un
occupied MOs are included in the active space of SAC-CI. CPU memory of
 700MB is specified with %mem to allocate electron repulsion integrals
 in core memory (all ERIs are stored on cpu). If the core memory is no
t enough for allocating all the repulsion integrals, according to the
available memory, the program will automatically divide the integral f
ile into appropriate number of files which are sequentially allocated
on the core memory. Experimental results and the results of LevelTwo c
alculations are compared in Part I-L of the SAC-CI Guide.
-----------------------------------------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
N                    2.12228   0.        0.
C                    2.90399   1.13165   0.
C                    2.43106   2.44892   0.
C                    1.08701   2.86082   0.
N                    0.        2.03212   0.
C                   -1.08701   2.86082   0.
C                   -2.43106   2.44892   0.
C                   -2.90399   1.13165   0.
N                   -2.12228   0.        0.
C                   -2.90399  -1.13165   0.
C                   -2.43106  -2.44892   0.
C                   -1.08701  -2.86082   0.
N                    0.       -2.03212   0.
C                    1.08701  -2.86082   0.
C                    2.43106  -2.44892   0.
C                    2.90399  -1.13165   0.
C                    4.27486  -0.69019   0.
C                    4.27486   0.69019   0.
H                    5.13171   1.35349   0.
```

H	5.13171	-1.35349	0.
H	3.1887	-3.22901	0.
C	0.68235	-4.26883	0.
C	-0.68235	-4.26883	0.
H	-1.35712	-5.11834	0.
H	1.35712	-5.11834	0.
H	-3.1887	-3.22901	0.
C	-4.27486	-0.69019	0.
C	-4.27486	0.69019	0.
H	-5.13171	1.35349	0.
H	-5.13171	-1.35349	0.
H	-1.10627	0.	0.
H	-3.1887	3.22901	0.
C	-0.68235	4.26883	0.
C	0.68235	4.26883	0.
H	1.35712	5.11834	0.
H	-1.35712	5.11834	0.
H	3.1887	3.22901	0.
H	1.10627	0.	0.

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.122283	0.000000	0.000000
2	6	0	2.903991	1.131654	0.000000
3	6	0	2.431060	2.448915	0.000000
4	6	0	1.087013	2.860819	0.000000
5	7	0	0.000000	2.032117	0.000000
6	6	0	-1.087013	2.860819	0.000000
7	6	0	-2.431060	2.448915	0.000000
8	6	0	-2.903991	1.131654	0.000000
9	7	0	-2.122283	0.000000	0.000000
10	6	0	-2.903991	-1.131654	0.000000
11	6	0	-2.431060	-2.448915	0.000000
12	6	0	-1.087013	-2.860819	0.000000
13	7	0	0.000000	-2.032117	0.000000
14	6	0	1.087013	-2.860819	0.000000
15	6	0	2.431060	-2.448915	0.000000
16	6	0	2.903991	-1.131654	0.000000
17	6	0	4.274858	-0.690194	0.000000
18	6	0	4.274858	0.690194	0.000000
19	1	0	5.131714	1.353489	0.000000
20	1	0	5.131714	-1.353489	0.000000
21	1	0	3.188699	-3.229008	0.000000
22	6	0	0.682348	-4.268828	0.000000
23	6	0	-0.682348	-4.268828	0.000000
24	1	0	-1.357121	-5.118337	0.000000

Nuclear coordinates for free-base porphin given in the Gaussian

25	1	0	1.357121	-5.118337	0.000000
26	1	0	-3.188699	-3.229008	0.000000
27	6	0	-4.274858	-0.690194	0.000000
28	6	0	-4.274858	0.690194	0.000000
29	1	0	-5.131714	1.353489	0.000000
30	1	0	-5.131714	-1.353489	0.000000
31	1	0	-1.106269	0.000000	0.000000
32	1	0	-3.188699	3.229008	0.000000
33	6	0	-0.682348	4.268828	0.000000
34	6	0	0.682348	4.268828	0.000000
35	1	0	1.357121	5.118337	0.000000
36	1	0	-1.357121	5.118337	0.000000
37	1	0	3.188699	3.229008	0.000000
38	1	0	1.106269	0.000000	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	N	0.000000				
2	C	1.375394	0.000000			
3	C	2.468305	1.399586	0.000000		
4	C	3.042379	2.508270	1.405748	0.000000	
5	N	2.938296	3.040394	2.466531	1.366874	0.000000
6	C	4.299287	4.349497	3.542104	2.174026	1.366874
7	C	5.170118	5.495266	4.862120	3.542104	2.466531
8	C	5.152094	5.807982	5.495266	4.349497	3.040394
9	N	4.244566	5.152094	5.170118	4.299287	2.938296
10	C	5.152094	6.233395	6.425204	5.645171	4.294486
11	C	5.170118	6.425204	6.901373	6.369467	5.098009
12	C	4.299287	5.645171	6.369467	6.120746	5.012227
13	N	2.938296	4.294486	5.098009	5.012227	4.064234
14	C	3.042379	4.386485	5.477202	5.721638	5.012227
15	C	2.468305	3.611667	4.897830	5.477202	5.098009
16	C	1.375394	2.263308	3.611667	4.386485	4.294486
17	C	2.260519	2.280001	3.640549	4.772007	5.068075
18	C	2.260519	1.440196	2.548076	3.856678	4.480532
19	H	3.299789	2.238741	2.914359	4.316439	5.176391
20	H	3.299789	3.337467	4.663883	5.841233	6.147912
21	H	3.400549	4.369946	5.728248	6.442288	6.152011
22	C	4.505142	5.839598	6.941618	7.141122	6.337784
23	C	5.107724	6.482826	7.404146	7.345918	6.337784
24	H	6.188992	7.564355	8.462483	8.345102	7.278102
25	H	5.175215	6.438571	7.643078	7.983726	7.278102
26	H	6.215547	7.492412	7.988773	7.440948	6.152011
27	C	6.434266	7.406416	7.404279	6.431124	5.068075
28	C	6.434266	7.192410	6.932708	5.784572	4.480532
29	H	7.379187	8.038766	7.641695	6.398797	5.176391
30	H	7.379187	8.411212	8.464858	7.512187	6.147912
31	H	3.228552	4.166872	4.302311	3.604826	2.313727
32	H	6.215547	6.443583	5.673644	4.291535	3.405929

33	C	5.107724	4.764839	3.606299	2.261223	2.338477
34	C	4.505142	3.844159	2.523901	1.465006	2.338477
35	H	5.175215	4.276266	2.877353	2.273620	3.371429
36	H	6.188992	5.835299	4.634234	3.327188	3.371429
37	H	3.400549	2.116590	1.087457	2.133693	3.405929
38	H	1.016014	2.124252	2.784287	2.860884	2.313727
		6	7	8	9	10
6	C	0.000000				
7	C	1.405748	0.000000			
8	C	2.508270	1.399586	0.000000		
9	N	3.042379	2.468305	1.375394	0.000000	
10	C	4.386485	3.611667	2.263308	1.375394	0.000000
11	C	5.477202	4.897830	3.611667	2.468305	1.399586
12	C	5.721638	5.477202	4.386485	3.042379	2.508270
13	N	5.012227	5.098009	4.294486	2.938296	3.040394
14	C	6.120746	6.369467	5.645171	4.299287	4.349497
15	C	6.369467	6.901373	6.425204	5.170118	5.495266
16	C	5.645171	6.425204	6.233395	5.152094	5.807982
17	C	6.431124	7.404279	7.406416	6.434266	7.192410
18	C	5.784572	6.932708	7.192410	6.434266	7.406416
19	H	6.398797	7.641695	8.038766	7.379187	8.411212
20	H	7.512187	8.464858	8.411212	7.379187	8.038766
21	H	7.440948	7.988773	7.492412	6.215547	6.443583
22	C	7.345918	7.404146	6.482826	5.107724	4.764839
23	C	7.141122	6.941618	5.839598	4.505142	3.844159
24	H	7.983726	7.643078	6.438571	5.175215	4.276266
25	H	8.345102	8.462483	7.564355	6.188992	5.835299
26	H	6.442288	5.728248	4.369946	3.400549	2.116590
27	C	4.772007	3.640549	2.280001	2.260519	1.440196
28	C	3.856678	2.548076	1.440196	2.260519	2.280001
29	H	4.316439	2.914359	2.238741	3.299789	3.337467
30	H	5.841233	4.663883	3.337467	3.299789	2.238741
31	H	2.860884	2.784287	2.124252	1.016014	2.124252
32	H	2.133693	1.087457	2.116590	3.400549	4.369946
33	C	1.465006	2.523901	3.844159	4.505142	5.839598
34	C	2.261223	3.606299	4.764839	5.107724	6.482826
35	H	3.327188	4.634234	5.835299	6.188992	7.564355
36	H	2.273620	2.877353	4.276266	5.175215	6.438571
37	H	4.291535	5.673644	6.443583	6.215547	7.492412
38	H	3.604826	4.302311	4.166872	3.228552	4.166872
		11	12	13	14	15
11	C	0.000000				
12	C	1.405748	0.000000			
13	N	2.466531	1.366874	0.000000		
14	C	3.542104	2.174026	1.366874	0.000000	
15	C	4.862120	3.542104	2.466531	1.405748	0.000000
16	C	5.495266	4.349497	3.040394	2.508270	1.399586
17	C	6.932708	5.784572	4.480532	3.856678	2.548076
18	C	7.404279	6.431124	5.068075	4.772007	3.640549

19	H	8.464858	7.512187	6.147912	5.841233	4.663883
20	H	7.641695	6.398797	5.176391	4.316439	2.914359
21	H	5.673644	4.291535	3.405929	2.133693	1.087457
22	C	3.606299	2.261223	2.338477	1.465006	2.523901
23	C	2.523901	1.465006	2.338477	2.261223	3.606299
24	H	2.877353	2.273620	3.371429	3.327188	4.634234
25	H	4.634234	3.327188	3.371429	2.273620	2.877353
26	H	1.087457	2.133693	3.405929	4.291535	5.673644
27	C	2.548076	3.856678	4.480532	5.784572	6.932708
28	C	3.640549	4.772007	5.068075	6.431124	7.404279
29	H	4.663883	5.841233	6.147912	7.512187	8.464858
30	H	2.914359	4.316439	5.176391	6.398797	7.641695
31	H	2.784287	2.860884	2.313727	3.604826	4.302311
32	H	5.728248	6.442288	6.152011	7.440948	7.988773
33	C	6.941618	7.141122	6.337784	7.345918	7.404146
34	C	7.404146	7.345918	6.337784	7.141122	6.941618
35	H	8.462483	8.345102	7.278102	7.983726	7.643078
36	H	7.643078	7.983726	7.278102	8.345102	8.462483
37	H	7.988773	7.440948	6.152011	6.442288	5.728248
38	H	4.302311	3.604826	2.313727	2.860884	2.784287
		16	17	18	19	20
16	C	0.000000				
17	C	1.440196	0.000000			
18	C	2.280001	1.380388	0.000000		
19	H	3.337467	2.216042	1.083588	0.000000	
20	H	2.238741	1.083588	2.216042	2.706978	0.000000
21	H	2.116590	2.761398	4.066926	4.977408	2.700533
22	C	3.844159	5.070774	6.123563	7.169889	5.319404
23	C	4.764839	6.113960	7.011832	8.087878	6.504039
24	H	5.835299	7.164331	8.090625	9.164579	7.501937
25	H	4.276266	5.302984	6.500171	7.492135	5.331194
26	H	6.443583	7.883544	8.429996	9.498871	8.529176
27	C	7.192410	8.549716	8.660434	9.626019	9.429929
28	C	7.406416	8.660434	8.549716	9.429929	9.626019
29	H	8.411212	9.626019	9.429929	10.263428	10.614409
30	H	8.038766	9.429929	9.626019	10.614409	10.263428
31	H	4.166872	5.425209	5.425209	6.383131	6.383131
32	H	7.492412	8.429996	7.883544	8.529176	9.498871
33	C	6.482826	7.011832	6.113960	6.504039	8.087878
34	C	5.839598	6.123563	5.070774	5.319404	7.169889
35	H	6.438571	6.500171	5.302984	5.331194	7.492135
36	H	7.564355	8.090625	7.164331	7.501937	9.164579
37	H	4.369946	4.066926	2.761398	2.700533	4.977408
38	H	2.124252	3.242888	3.242888	4.246898	4.246898
		21	22	23	24	25
21	H	0.000000				
22	C	2.713489	0.000000			
23	C	4.008270	1.364696	0.000000		
24	H	4.922809	2.209321	1.084889	0.000000	

25	H	2.631395	1.084889	2.209321	2.714242	0.000000
26	H	6.377398	4.008270	2.713489	2.631395	4.922809
27	C	7.883544	6.113960	5.070774	5.302984	7.164331
28	C	8.429996	7.011832	6.123563	6.500171	8.090625
29	H	9.498871	8.087878	7.169889	7.492135	9.164579
30	H	8.529176	6.504039	5.319404	5.331194	7.501937
31	H	5.373383	4.628395	4.289825	5.124480	5.680287
32	H	9.076187	8.438160	7.905652	8.545926	9.504875
33	C	8.438160	8.646038	8.537656	9.411386	9.606160
34	C	7.905652	8.537656	8.646038	9.606160	9.411386
35	H	8.545926	9.411386	9.606160	10.590402	10.236674
36	H	9.504875	9.606160	9.411386	10.236674	10.590402
37	H	6.458016	7.905652	8.438160	9.504875	8.545926
38	H	3.842266	4.289825	4.628395	5.680287	5.124480

		26	27	28	29	30
26	H	0.000000				
27	C	2.761398	0.000000			
28	C	4.066926	1.380388	0.000000		
29	H	4.977408	2.216042	1.083588	0.000000	
30	H	2.700533	1.083588	2.216042	2.706978	0.000000
31	H	3.842266	3.242888	3.242888	4.246898	4.246898
32	H	6.458016	4.066926	2.761398	2.700533	4.977408
33	C	7.905652	6.123563	5.070774	5.319404	7.169889
34	C	8.438160	7.011832	6.113960	6.504039	8.087878
35	H	9.504875	8.090625	7.164331	7.501937	9.164579
36	H	8.545926	6.500171	5.302984	5.331194	7.492135
37	H	9.076187	8.429996	7.883544	8.529176	9.498871
38	H	5.373383	5.425209	5.425209	6.383131	6.383131

		31	32	33	34	35
31	H	0.000000				
32	H	3.842266	0.000000			
33	C	4.289825	2.713489	0.000000		
34	C	4.628395	4.008270	1.364696	0.000000	
35	H	5.680287	4.922809	2.209321	1.084889	0.000000
36	H	5.124480	2.631395	1.084889	2.209321	2.714242
37	H	5.373383	6.377398	4.008270	2.713489	2.631395
38	H	2.212538	5.373383	4.628395	4.289825	5.124480

		36	37	38
36	H	0.000000		
37	H	4.922809	0.000000	
38	H	5.680287	3.842266	0.000000

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Stoichiometry    C20H14N4
Framework group  D2H[C2'(N.N),C2"(NH.HN),SG(C20H12)]
Deg. of freedom    19
Full point group                 D2H     NOp   8
Largest Abelian subgroup         D2H     NOp   8
Largest concise Abelian subgroup D2      NOp   4
                         Standard orientation:
---------------------------------------------------------------------
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	2.122283
2	6	0	0.000000	1.131654	2.903991
3	6	0	0.000000	2.448915	2.431060
4	6	0	0.000000	2.860819	1.087013
5	7	0	0.000000	2.032117	0.000000
6	6	0	0.000000	2.860819	-1.087013
7	6	0	0.000000	2.448915	-2.431060
8	6	0	0.000000	1.131654	-2.903991
9	7	0	0.000000	0.000000	-2.122283
10	6	0	0.000000	-1.131654	-2.903991
11	6	0	0.000000	-2.448915	-2.431060
12	6	0	0.000000	-2.860819	-1.087013
13	7	0	0.000000	-2.032117	0.000000
14	6	0	0.000000	-2.860819	1.087013
15	6	0	0.000000	-2.448915	2.431060
16	6	0	0.000000	-1.131654	2.903991
17	6	0	0.000000	-0.690194	4.274858
18	6	0	0.000000	0.690194	4.274858
19	1	0	0.000000	1.353489	5.131714
20	1	0	0.000000	-1.353489	5.131714
21	1	0	0.000000	-3.229008	3.188699
22	6	0	0.000000	-4.268828	0.682348
23	6	0	0.000000	-4.268828	-0.682348
24	1	0	0.000000	-5.118337	-1.357121
25	1	0	0.000000	-5.118337	1.357121
26	1	0	0.000000	-3.229008	-3.188699
27	6	0	0.000000	-0.690194	-4.274858
28	6	0	0.000000	0.690194	-4.274858
29	1	0	0.000000	1.353489	-5.131714
30	1	0	0.000000	-1.353489	-5.131714
31	1	0	0.000000	0.000000	-1.106269
32	1	0	0.000000	3.229008	-3.188699
33	6	0	0.000000	4.268828	-0.682348
34	6	0	0.000000	4.268828	0.682348
35	1	0	0.000000	5.118337	1.357121
36	1	0	0.000000	5.118337	-1.357121
37	1	0	0.000000	3.229008	3.188699
38	1	0	0.000000	0.000000	1.106269

Nuclear coordinates used in the actual calculation

```
Rotational constants (GHZ):      0.2645376      0.2621401      0.1316667
General basis read from cards:  (5D, 7F)
There are    60 symmetry adapted basis functions of AG  symmetry.
There are    12 symmetry adapted basis functions of B1G symmetry.
There are    12 symmetry adapted basis functions of B2G symmetry.
There are    50 symmetry adapted basis functions of B3G symmetry.
There are    10 symmetry adapted basis functions of AU  symmetry.
```

```
There are    56 symmetry adapted basis functions of B1U symmetry.
There are    54 symmetry adapted basis functions of B2U symmetry.
There are    14 symmetry adapted basis functions of B3U symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
  268 basis functions,   632 primitive gaussians,   268 cartesian basis functions
   81 alpha electrons       81 beta electrons
      nuclear repulsion energy      1847.4556980092 Hartrees.
NAtoms=   38 NActive=   38 NUniq=   11 SFac= 5.66D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=   268 RedAO= T  NBF=    60    12    12    50    10    56    54    14
NBsUse=   268 1.00D-06 NBFU=    60    12    12    50    10    56    54    14
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.20D-01 ExpMax= 3.66D+03 ExpMxC= 5.45D+02 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=         1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Initial guess orbital symmetries:
      Occupied  (B1U) (AG) (B2U) (AG) (B1U) (AG) (B3G) (B1U) (B2U)
                (AG) (B2U) (AG) (B3G) (B2U) (B3G) (B1U) (B1U)
                (B3G) (B2U) (AG) (B2U) (B3G) (B1U) (AG) (AG) (B1U)
                (B2U) (AG) (B3G) (B2U) (B1U) (AG) (B1U) (AG) (B2U)
                (AG) (B3G) (B2U) (B1U) (AG) (B3G) (B1U) (B2U)
                (AG) (B3G) (B1U) (B3G) (B2U) (AG) (B2U) (B1U)
                (B3G) (AG) (AG) (B1U) (B2U) (B1U) (AG) (B3U) (B3G)
                (AG) (B2G) (B2U) (B1G) (B1U) (B2U) (B1U) (B3U)
                (B3G) (B3G) (AU) (B1G) (B2U) (B2G) (AG) (B3U)
                (B2G) (B3U) (B1G) (AU) (B3U)
      Virtual   (B2G) (B1G) (AU) (B3U) (B2G) (B1G) (AU) (AU) (B2G)
                (B1G) (B3U) (AG) (AG) (B1U) (B2U) (B3G) (B2U)
                (B1U) (AG) (B2U) (B3G) (B1U) (AG) (B3G) (AG) (B1U)
                (B2U) (B3G) (AG) (AG) (B3G) (B1U) (B2U) (B1U)
                (B2U) (AG) (B1U) (B2U) (B1U) (AG) (B3G) (B2U)
                (B3U) (B1U) (AG) (B2G) (B1G) (B3G) (B2U) (AU)
                (B3G) (B3U) (B1U) (B3G) (AG) (B3U) (B2G) (B1G)
                (B3G) (B2U) (B2G) (B1G) (AG) (B1U) (AG) (B2U)
                (B1U) (AU) (AG) (B2U) (B3G) (B1U) (AU) (B3G) (B2U)
                (B3U) (AG) (B1U) (B1U) (B3G) (B3U) (B2U) (B3G)
                (AG) (B1G) (B2G) (B1U) (B2U) (AG) (B2G) (B1G)
                (B3U) (AU) (B3G) (B2U) (B1U) (AU) (B3G) (B2U)
                (B1U) (AG) (AG) (B2U) (B3G) (B1U) (AG) (B2G) (B1G)
                (B2U) (B3G) (B3U) (B3G) (B3G) (B2U) (B1U) (B3G)
                (AG) (B2U) (B1U) (B1U) (AG) (B3G) (B2U) (AG) (B1U)
                (B2U) (AG) (B1U) (B3G) (B2U) (AG) (B3G) (B2U)
                (B1U) (AG) (B1U) (B3G) (AG) (B2U) (B3G) (B1U)
                (B3G) (B1U) (B2U) (AG) (AG) (B2U) (B1U) (B3G)
                (AG) (AG) (B3G) (B1U) (B2U) (B1U) (B3G) (B2U)
                (B3G) (AG) (B1U) (AG) (B1U) (B2U) (AG) (B2U) (B1U)
                (B3G) (B2U) (AG) (B1U) (B3G) (AG) (B2U) (B1U)
```

```
                (AG) (B3G) (B1U) (B2U) (AG) (B3G) (B1U) (B2U)
                (B3G) (AG) (AG) (B1U) (B2U)
The electronic state of the initial guess is 1-AG.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
SCF Done:  E(RHF) =  -982.925406060     A.U. after   16 cycles
           Convg  =    0.7737D-08             -V/T =  2.0010
           S**2   =   0.0000
Range of M.O.s used for correlation:    25   244
NBasis=   268 NAE=    81 NBE=    81 NFC=    24 NFV=    24
NROrb=    220 NOA=    57 NOB=    57 NVA=   163 NVB=   163
Semi-Direct transformation.
ModeAB=           4 MOrb=           220 LenV=      86643005
LASXX=     40755181 LTotXX=    40755181 LenRXX=    40755181
LTotAB=           0 MaxLAS=   179189010 LenRXY=           0
NonZer=    81510362 LenScr=   123014144 LnRSAI=   356756400
LnScr1=   539029504 LExtra=           0 Total=   1059555229
MaxDsk=          -1 SrtSym=           T ITran=            5
JobTyp=0 Pass  1:  I=   1 to 220.
--------------------------------------------------------------------
####################################################################
--------------------------------------------------------------------
              SAC/SAC-CI Program Combined with GAUSSIAN
                          for Calculating
        Ground, Excited, Ionized, and Electron-Attached States
                              and
            Singlet, Doublet, Triplet, Quartet, Quintet,
                  Sextet, and Septet Spin States
                              and
                 Their Analytical Energy Gradients
                        coded originally by
                         Hiroshi Nakatsuji
                          and extended by
 H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa,
      M. Ishida, T. Nakajima, Y. Honda, O. Kitao, and H. Nakai
                                at
                 Department of Hydrocarbon Chemistry,
               Division of Molecular Engineering, and
      Department of Synthetic Chemistry & Biological Chemistry,
                  Graduate School of Engineering,
                         Kyoto University,
                       Kyoto 606-8501, Japan
--------------------------------------------------------------------
####################################################################
--------------------------------------------------------------------
```

Hartree-Fock SCF energy.

AO to MO transformation of two-electron repulsion integrals

Beginning of the SAC-CI part of the program

```
No. of INTEGRALS =  40755181 NBLK =     25471 KOUNT =      1581
##############################################################################
    Singles-Doubles (SD) SAC/SAC-CI  (SAC-CI SD-R)
##############################################################################
================================================================
  STEP #PRES#  Generation of Linked Operators and Selection
================================================================
== States to be calculated ==
           AG   B1G  B2G  B3G  AU   B1U  B2U  B3U
SINGLET    Yes  Yes  Yes  Yes  Yes  Yes  Yes  Yes
TRIPLET    No   No   No   No   No   No   No   No
IONIZED    No   No   No   No   No   No   No   No
ANIONIZED  No   No   No   No   No   No   No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  0,  0,  0,  0,  4,  4,  1)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelOne #
  EThreS2 (Lambda_G)=  0.100D-04(au)   EThreR2 (Lambda_E)=  0.100D-05(au)
****************************
        SINGLET STATE
****************************
----------------------------------------------------------------
LINKED OPERATORS FOR SAC:    SYMMETRY = AG  GROUND STATE
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE          1527     5919374      5920901
    AFTER           1527       25867        27395
----------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.090236
      81 ->  83     0.69839       80 ->  82     0.68629
      74 ->  84    -0.10751
    ##   2-nd state ##       energy (au) =       0.165420
      81 ->  83     0.58232       80 ->  82    -0.56315
      78 ->  82    -0.50620       79 ->  84    -0.20660
    ##   3-th state ##       energy (au) =       0.194606
      78 ->  82     0.77704       80 ->  82    -0.40966
      81 ->  83     0.34947       79 ->  84     0.23975
    ##   4-th state ##       energy (au) =       0.249786
      75 ->  82     0.94660       76 ->  85    -0.17356
      81 ->  87     0.13554       75 ->  86    -0.10811
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE          1526     5914722      5916248
    AFTER           1526       60592        62118
----------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.095276
```

Number of the linked operators for single- and double- excitation operators before and after the perturbation selection

Main configurations of the reference SECI calculation used for the perturbation selection step. For example, the first excited state in singlet B_{1u} symmetry is the transition from 81-th MO to 83-th MO and from 80-th MO to 82-th MO, and their CI coefficient is about 0.70 and 0.69, respectively.

```
      81 ->  82     0.72368       80 ->  83    -0.66040
      77 ->  84    -0.11433
    ##   2-nd state ##       energy (au) =       0.173907
      80 ->  83     0.70832       81 ->  82     0.64382
      78 ->  83     0.14567
    ##   3-th state ##       energy (au) =       0.216814
      78 ->  83     0.81388       75 ->  83     0.49472
      76 ->  84     0.19959       79 ->  85     0.11404
    ##   4-th state ##       energy (au) =       0.230507
      75 ->  83     0.78121       78 ->  83    -0.50706
      76 ->  84     0.21917       80 ->  83     0.12920
      81 ->  82     0.11308       77 ->  84     0.11120
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE          1518     5914574      5916092
    AFTER           1518       57253        58771
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3U EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.236707
      72 ->  83     0.89222       73 ->  85    -0.30145
      72 ->  87    -0.18874       72 ->  99     0.18491
      73 -> 101    -0.13895
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE           806     4875766      4876572
    AFTER            806       23547        24353
================================================================
  STEP #CIMX#  CI matrix elements         ### SINGLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-03
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   AG    CONVERGED
Solution for Singlet   B1U   CONVERGED
Solution for Singlet   B2U   CONVERGED
Solution for Singlet   B3U   CONVERGED
================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
================================================================
Threshold for S2 operator (CThreULS2G) 0.500D-02
================================================================
  STEP #SAC#  Solution of SAC equation
================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-05
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
```

```
Solution for SAC equation converged
*******************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*******************************************
HF ENERGY     =    -982.925406 (AU)
SAC-NV  ENERGY=      -0.481382 (AU)
TOTAL ENERGY  =    -983.406788 (AU)
SAC-NV  coefficients (|C|>=0.03)
*SINGLE EXCITATION
*DOUBLE EXCITATION
      81   83   80   82      0.06722        80   83   80   83     -0.05235
      80   84   77   83     -0.04842        81   82   81   82     -0.04508
      81   84   77   82      0.04057        81   82   80   83     -0.03746
      78   86   78   82     -0.03302        80   82   80   82     -0.03242
      81   85   74   82     -0.03121        81   83   81   83     -0.03101
      79   86   78   84     -0.03086        80   83   77   84     -0.03055
      75   87   75   83     -0.03023
Hartree-Fock configuration   1.00000
=====================================================================
  STEP #ULINTS#  Unlinked integral for Singlet Excited State (SAC-CI)
=====================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
=================================================================
  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
=================================================
Threshold for density convergence (DConvDiag) .100D-
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   B1U   CONVERGED
Solution for Singlet   B2U   CONVERGED
Solution for Singlet   B3U   CONVERGED
**********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
**********************************************
*****************************************************************************
Singlet       B1U     ***********************************************************
###   1-st  ###          ---   1st state in this spin multiplicity ---
    Total energy       in au =    -983.341835
    Correlation energy in au =      -0.416429
    Excitation energy  in au =       0.064953    in eV =       1.767464
  *SINGLE EXCITATION
      80   82     0.71892        81   83     0.60917
      78   82     0.09900        79   84     0.04487
  *DOUBLE EXCITATION
      80   82   77   82    -0.10529        80   84   80   83     0.09720
      81   82   80   84     0.09050        81   83   77   82     0.08838
      81   84   80   82     0.08746        81   82   77   83     0.08233
      80   83   77   83     0.07932        81   84   81   83    -0.06736
      81   83   74   83    -0.06477        80   83   79   82    -0.05373
```

Result of SAC calculation. Hartree-Fock (HF) energy, SAC-NV energy (correlation energy obtained with the SAC method), and the SAC-NV coefficients are shown. HF configuration always has 1.00 in the SAC wave function.

Result of SAC-CI calculation. Total energy, correlation energy (HF energy as the reference), excitation energy (SAC total energy as the reference), and the SAC-CI coefficients are shown. For example, the first excited state in singlet B_{1u} symmetry is the excitation from 80-th MO to 82-th MO and from 81-th MO to 83-th MO, and their excitation energy is 1.77 eV.

```
     81   83   80   85     0.05136        81   85   81   82     0.05126
     80   83   74   82     0.04834        81   85   80   83     0.04720
     80   85   80   82    -0.04691        81   83   79   83     0.04672
     80   82   76   82     0.04657        81   82   79   82    -0.03641
     81   87   76   82     0.03312        81   88   75   82     0.03019
###   2-nd  ###           ---   3rd state in this spin multiplicity ---
   Total energy       in au =    -983.275396
   Correlation energy in au =      -0.349990
   Excitation energy  in au =       0.131392    in eV =       3.575369
  *SINGLE EXCITATION
     81   83    -0.65043        80   82     0.47493
     78   82     0.45921        75   82    -0.14634
     79   84     0.09911
  *DOUBLE EXCITATION
     81   82   79   82    -0.11164        80   83   79   82    -0.09978
     81   82   77   83    -0.09387        81   84   81   83     0.08996
     81   83   74   83     0.07342        81   83   79   83    -0.06465
     81   84   80   82    -0.06398        80   82   77   82    -0.06237
     80   84   80   83     0.05462        80   82   78   85    -0.04725
     81   84   78   82    -0.04530        80   85   80   82    -0.04248
     80   82   76   82     0.04074        81   85   81   82    -0.03704
     81   82   76   83     0.03616        81   83   77   82    -0.03461
     81   85   80   83    -0.03421        80   83   77   83    -0.03160
     81   83   80   85     0.03003
###   3-rd  ###           ---   5th state in this spin multiplicity ---
   Total energy       in au =    -983.254585
   Correlation energy in au =      -0.329179
   Excitation energy  in au =       0.152203    in eV =       4.141650
  *SINGLE EXCITATION
     78   82    -0.78656        80   82     0.34894
     81   83    -0.27542        75   82    -0.18588
     79   84    -0.08668        67   82     0.07498
     78   86     0.04378        81   87    -0.03029
  *DOUBLE EXCITATION
     81   82   79   82     0.20657        81   84   78   82     0.11962
     81   82   74   82     0.11309        80   82   76   82     0.08640
     80   82   77   82    -0.07001        80   83   79   82     0.06409
     80   83   74   82     0.06337        80   83   78   84    -0.06160
     81   86   79   82     0.05996        81   88   78   82    -0.05895
     80   84   80   83     0.05398        81   83   78   85    -0.05317
     81   83   76   82    -0.05058        80   82   78   85     0.04945
     81   84   75   82    -0.04552        81   82   77   83    -0.03522
     81   87   77   82    -0.03375        81   85   81   82    -0.03314
     81   82   75   84    -0.03245        81   84   81   83     0.03153
###   4-th  ###           ---   9th state in this spin multiplicity ---
   Total energy       in au =    -983.225878
   Correlation energy in au =      -0.300472
   Excitation energy  in au =       0.180910    in eV =       4.922804
  *SINGLE EXCITATION
```

```
     75   82     0.88224        81   83    -0.16065
     80   82     0.15941        81   87     0.08630
     78   82    -0.08561
  *DOUBLE EXCITATION
     81   83   76   82     0.17890        80   82   76   82    -0.14292
     81   84   75   82     0.13581        81   82   75   84     0.11366
     81   83   77   82     0.10975        80   83   75   84     0.08999
     80   82   77   82    -0.08117        80   85   75   82     0.07513
     75   82   74   83    -0.07421        77   82   75   82    -0.07321
     81   88   75   82     0.06999        81   82   79   82     0.06990
     81   87   76   82     0.06134        81   82   76   83     0.05975
     81   84   78   82     0.05951        81   87   77   82     0.05110
     81   82   74   82     0.04088        81   82   80   84     0.03435
     81   82   75   88     0.03181        81   84   80   82     0.03115
     81   82   76   87     0.03108
*******************************************************************************
Singlet       B2U     ******************************************************
###   1-st  ###           ---   2nd state in this spin multiplicity ---
    Total energy       in au =    -983.324213
    Correlation energy in au =      -0.398807
    Excitation energy  in au =       0.082575    in eV =       2.246974
  *SINGLE EXCITATION
     80   83     0.69824        81   82    -0.64738
     75   83    -0.10118
  *DOUBLE EXCITATION
     80   83   74   83     0.09652        81   83   80   84    -0.08068
     80   84   80   82     0.08051        81   84   80   83    -0.07885
     81   82   74   83     0.07472        81   83   74   82     0.07258
     80   82   74   82    -0.06086        81   84   81   82    -0.05863
     81   82   77   82    -0.05714        80   83   79   83    -0.05654
     81   82   76   82     0.04678        81   85   81   83    -0.04252
     80   82   77   83    -0.04121        80   82   76   83     0.03681
     80   83   77   82    -0.03591
###   2-nd  ###           ---   4th state in this spin multiplicity ---
    Total energy       in au =    -983.270599
    Correlation energy in au =      -0.345193
    Excitation energy  in au =       0.136189    in eV =       3.705885
  *SINGLE EXCITATION
     81   82     0.66051        80   83     0.59917
     78   83     0.26191        75   83    -0.13455
     81   86     0.04934
  *DOUBLE EXCITATION
     80   83   79   83    -0.10742        80   84   80   82     0.09774
     81   83   74   82    -0.08712        80   83   74   83     0.08554
     81   84   81   82     0.07645        81   83   77   83     0.06437
     80   83   77   82     0.06057        81   84   80   83     0.06028
     81   82   79   83    -0.05933        81   84   78   83    -0.05897
     81   82   77   82     0.05896        81   82   76   82    -0.05838
     81   85   81   83     0.05782        80   82   76   83     0.04963
```

```
     81   86   74   83    -0.04862        81   83   78   84    -0.03806
     81   82   74   83    -0.03130
###   3-rd  ###           ---   6th state in this spin multiplicity ---
   Total energy       in au =    -983.247675
   Correlation energy in au =      -0.322269
   Excitation energy  in au =       0.159113    in eV =       4.329687
  *SINGLE EXCITATION
     78   83     0.84223        75   83     0.30200
     81   82    -0.20566        80   83    -0.10164
     67   83    -0.06115        76   84     0.05784
  *DOUBLE EXCITATION
     81   82   79   83    -0.16660        80   83   79   83    -0.13360
     81   84   78   83    -0.12201        80   82   78   84     0.09809
     81   83   78   84    -0.09447        78   83   77   82     0.08201
     81   83   76   83     0.08067        80   82   76   83    -0.07807
     80   83   74   83    -0.06083        81   86   79   83    -0.05956
     81   82   74   83    -0.05630        81   88   78   83     0.05303
     81   83   79   82    -0.04899        81   84   75   83     0.04860
     80   83   63   83    -0.04754        80   85   75   83     0.03950
     80   83   75   85     0.03857        75   83   74   83    -0.03317
     78   82   77   83     0.03316        81   86   74   83    -0.03143
     80   84   78   82     0.03106
###   4-th  ###           ---   8th state in this spin multiplicity ---
   Total energy       in au =    -983.228396
   Correlation energy in au =      -0.302990
   Excitation energy  in au =       0.178392    in eV =       4.854296
  *SINGLE EXCITATION
     75   83    -0.85298        78   83     0.25444
     80   83    -0.20963        81   82    -0.09306
     76   84    -0.09242        58   83    -0.06154
     75   87     0.04331        67   83     0.03208
  *DOUBLE EXCITATION
     81   83   76   83    -0.18095        81   83   77   83    -0.14852
     80   82   76   83     0.10526        81   84   75   83    -0.10457
     80   83   75   85    -0.07761        80   83   79   83    -0.07542
     81   84   78   83    -0.07431        81   82   79   83    -0.07367
     75   83   74   83     0.06330        80   82   75   84    -0.06273
     81   88   75   83    -0.05796        80   82   77   83     0.05596
     80   85   75   83    -0.05555        81   87   76   83    -0.05264
     81   82   75   85    -0.05169        79   83   75   83    -0.04864
     81   82   74   83    -0.04641        81   83   78   84    -0.04466
     81   84   80   83    -0.04271        80   82   78   84     0.04234
     78   83   77   82     0.04220        80   84   80   82    -0.03943
     81   86   79   83    -0.03652
*****************************************************************************
Singlet       B3U     ***********************************************************
###   1-st  ###           ---   7th state in this spin multiplicity ---
   Total energy       in au =    -983.244252
   Correlation energy in au =      -0.318846
```

```
   Excitation energy  in au =       0.162537    in eV =       4.422846
  *SINGLE EXCITATION
      72   83     0.92666        73   85    -0.10396
      72   87    -0.07549
  *DOUBLE EXCITATION
      80   83   73   83     0.18409        81   82   73   83     0.12538
      80   85   72   83    -0.10399        80   82   72   84     0.08008
      80   99   73   83     0.07136        81   83   72   84    -0.06958
      77   82   72   83     0.06758        81   84   72   83    -0.06517
      80  101   72   83    -0.06465        80   87   73   83    -0.06345
      79   83   72   83    -0.05535        79   85   73   83     0.04761
================================================================
  STEP #DENS#  Density Calculation
================================================================
Transition density for SAC/SAC-CI (V)
Threshold for S2 operators (CThreDensULS2):  0.50D-02
Threshold for R1,R2 operators (CThreDensULR1):  0.10D+00
Only right vectors are used. (ILEFT=0)
--------------------------------------------------------------------------
Transition dipole moment of   singlet state from SAC ground state
--------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
--------------------------------------------------------------------------
   AG         0      0.0          Excitations are from this state.
   B1U        1      1.7675      0.0000      0.0000      0.1026      0.0005
   B1U        2      3.5754      0.0000      0.0000      3.6743      1.1826
   B1U        3      4.1416      0.0000      0.0000      2.7731      0.7803
   B1U        4      4.9228      0.0000      0.0000      1.8370      0.4070
   B2U        1      2.2470      0.0000      0.0355      0.0000      0.0001
   B2U        2      3.7059      0.0000     -4.3126      0.0000      1.6886
   B2U        3      4.3297      0.0000      1.6080      0.0000      0.2743
   B2U        4      4.8543      0.0000      1.5978      0.0000      0.3036
   B3U        1      4.4228     -0.1977      0.0000      0.0000      0.0042
--------------------------------------------------------------------------
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.

*********************************************************************

           Population analysis using the SCF density.

*********************************************************************

Orbital symmetries:
      Occupied  (AG) (B1U) (AG) (B2U) (B3G) (B2U) (AG) (B1U) (B3G)
                (B1U) (AG) (B2U) (AG) (B1U) (B3G) (B2U) (AG) (B1U)
                (B3G) (B2U) (AG) (B2U) (B3G) (B1U) (AG) (B1U)
                (B2U) (AG) (B3G) (B2U) (AG) (B1U) (B1U) (B2U)
```

Transition dipole moments and oscillator strengths of the excited states.are summarized. SAC w.f. is used for the ground state.

```
                (AG)  (AG)  (B3G)  (B2U)  (B1U)  (B3G)  (AG)  (B1U)  (B2U)
                (B3G)  (AG)  (B1U)  (B3G)  (B2U)  (AG)  (B2U)  (B1U)
                (AG)  (B1U)  (AG)  (B3G)  (B2U)  (B1U)  (B3U)  (B2G)
                (AG)  (B3G)  (B2U)  (B1G)  (AG)  (B2U)  (B1U)  (B3U)
                (B3G)  (B1U)  (B3G)  (AU)  (B2U)  (AG)  (B1G)  (B3U)
                (B2G)  (B2G)  (B3U)  (B1G)  (B3U)  (AU)
      Virtual   (B2G)  (B1G)  (AU)  (B3U)  (B2G)  (B1G)  (AU)  (AU)  (B2U)
                (B1U)  (AG)  (B3G)  (B2G)  (AG)  (B3G)  (B1U)  (AG)  (B1G)
                (B2U)  (B3U)  (B1U)  (B2U)  (AG)  (B3G)  (AG)  (B1U)
                (B2U)  (B1U)  (B3G)  (AG)  (B2U)  (AG)  (B1U)  (AG)  (B3G)
                (B2U)  (B1U)  (B2U)  (AG)  (B3G)  (AG)  (B3U)  (B1U)
                (B2G)  (B1G)  (B2U)  (B3G)  (B1U)  (B3G)  (B3U)  (B2U)
                (AU)  (B2U)  (B3G)  (B1U)  (B3U)  (B1U)  (B2G)  (B1G)
                (AG)  (B3G)  (B2G)  (B1G)  (AG)  (AU)  (B3G)  (AG)  (B1U)
                (B2U)  (B3U)  (B3G)  (AU)  (B2U)  (B3U)  (B1U)  (AG)
                (B2U)  (B1U)  (B3G)  (AG)  (B1G)  (AG)  (B2G)  (B1U)
                (B1G)  (B2U)  (B2G)  (AU)  (B2U)  (B1U)  (AG)  (AU)  (B3U)
                (B3G)  (B2U)  (B3G)  (B1U)  (B3G)  (AG)  (B2U)  (B2G)
                (B1U)  (AG)  (B3G)  (B2U)  (B1G)  (AG)  (B1U)  (B3G)
                (B2U)  (B3U)  (B3G)  (B1U)  (B2U)  (AG)  (B1U)  (B2U)
                (B3G)  (B3G)  (B3G)  (AG)  (B1U)  (B2U)  (B1U)  (B2U)
                (AG)  (B1U)  (AG)  (B2U)  (B3G)  (B3G)  (AG)  (B1U)  (B2U)
                (AG)  (B1U)  (B3G)  (AG)  (B2U)  (B3G)  (B1U)  (B3G)
                (B1U)  (B2U)  (AG)  (AG)  (B2U)  (B1U)  (B3G)  (AG)  (AG)
                (B3G)  (B1U)  (B2U)  (B3G)  (B1U)  (B2U)  (B3G)  (B1U)
                (AG)  (AG)  (B1U)  (B2U)  (AG)  (B2U)  (B1U)  (B3G)  (B2U)
                (AG)  (B1U)  (B3G)  (AG)  (B2U)  (B1U)  (AG)  (B3G)  (B1U)
                (B2U)  (AG)  (B3G)  (B1U)  (B2U)  (B3G)  (AG)  (AG)  (B1U)
                (B2U)
The electronic state is 1-AG.
Alpha  occ. eigenvalues --  -15.60276 -15.60276 -15.54668 -15.54667 -11.30852
Alpha  occ. eigenvalues --  -11.30852 -11.30848 -11.30848 -11.28637 -11.28636
Alpha  occ. eigenvalues --  -11.28633 -11.28633 -11.26606 -11.26606 -11.26604
Alpha  occ. eigenvalues --  -11.26604 -11.26603 -11.26603 -11.26474 -11.26474
Alpha  occ. eigenvalues --  -11.25125 -11.25125 -11.24982 -11.24982  -1.31824
Alpha  occ. eigenvalues --   -1.31615  -1.27554  -1.27222  -1.11014  -1.08305
Alpha  occ. eigenvalues --   -1.07830  -1.07695  -1.07034  -1.04361  -1.04324
Alpha  occ. eigenvalues --   -1.01247  -0.98619  -0.90998  -0.90089  -0.82715
Alpha  occ. eigenvalues --   -0.81686  -0.80427  -0.79578  -0.78799  -0.78383
Alpha  occ. eigenvalues --   -0.76431  -0.75621  -0.71883  -0.70302  -0.69183
Alpha  occ. eigenvalues --   -0.68782  -0.63684  -0.61900  -0.61516  -0.61506
Alpha  occ. eigenvalues --   -0.60270  -0.59989  -0.59973  -0.59275  -0.59159
Alpha  occ. eigenvalues --   -0.58592  -0.55889  -0.55433  -0.54886  -0.54544
Alpha  occ. eigenvalues --   -0.53730  -0.53715  -0.53077  -0.52695  -0.52667
Alpha  occ. eigenvalues --   -0.44521  -0.42381  -0.42112  -0.38664  -0.38054
Alpha  occ. eigenvalues --   -0.37981  -0.37449  -0.34466  -0.33865  -0.24387
Alpha  occ. eigenvalues --   -0.23809
Alpha virt. eigenvalues --    0.00025   0.00201   0.10139   0.18815   0.20556
Alpha virt. eigenvalues --    0.20855   0.22283   0.25131   0.26548   0.26641
```

```
Alpha virt. eigenvalues --    0.26728   0.26980   0.27671   0.27768   0.28190
Alpha virt. eigenvalues --    0.28618   0.28778   0.29451   0.29657   0.29786
Alpha virt. eigenvalues --    0.30121   0.30224   0.33281   0.33346   0.34312
Alpha virt. eigenvalues --    0.35593   0.35600   0.36805   0.37156   0.38222
Alpha virt. eigenvalues --    0.39205   0.39281   0.40537   0.41109   0.41989
Alpha virt. eigenvalues --    0.42478   0.42628   0.42664   0.44075   0.47313
Alpha virt. eigenvalues --    0.48489   0.48671   0.48704   0.49555   0.50405
Alpha virt. eigenvalues --    0.50429   0.51758   0.52228   0.52549   0.52612
Alpha virt. eigenvalues --    0.53058   0.54197   0.55491   0.55732   0.55847
Alpha virt. eigenvalues --    0.56052   0.56375   0.56418   0.56520   0.57153
Alpha virt. eigenvalues --    0.58736   0.60407   0.60526   0.60923   0.62174
Alpha virt. eigenvalues --    0.62620   0.62986   0.63209   0.63505   0.64530
Alpha virt. eigenvalues --    0.65018   0.65023   0.65407   0.65934   0.67806
Alpha virt. eigenvalues --    0.68069   0.68122   0.69371   0.69611   0.70574
Alpha virt. eigenvalues --    0.70628   0.71277   0.71406   0.72577   0.74379
Alpha virt. eigenvalues --    0.74429   0.74520   0.78327   0.78328   0.78599
Alpha virt. eigenvalues --    0.79050   0.80506   0.80849   0.83563   0.85796
Alpha virt. eigenvalues --    0.87631   0.88015   0.88424   0.89539   0.90075
Alpha virt. eigenvalues --    0.91790   0.92433   0.94146   0.95650   0.96424
Alpha virt. eigenvalues --    0.96677   0.96954   0.99035   0.99648   0.99941
Alpha virt. eigenvalues --    1.00271   1.01116   1.02460   1.03230   1.03621
Alpha virt. eigenvalues --    1.06565   1.06628   1.06906   1.08956   1.17365
Alpha virt. eigenvalues --    1.17673   1.18280   1.19106   1.22230   1.22550
Alpha virt. eigenvalues --    1.23038   1.24602   1.25377   1.27714   1.28522
Alpha virt. eigenvalues --    1.29667   1.31013   1.32666   1.33192   1.35341
Alpha virt. eigenvalues --    1.35908   1.36316   1.36681   1.38618   1.39855
Alpha virt. eigenvalues --    1.40518   1.41354   1.45045   1.45764   1.45864
Alpha virt. eigenvalues --    1.46979   1.48437   1.53920   1.64336   1.69160
Alpha virt. eigenvalues --    1.69979   1.70358   1.70481   1.70761   1.74673
Alpha virt. eigenvalues --    1.74774   1.74835   1.79274   1.86443   1.86724
Alpha virt. eigenvalues --    1.92528   1.92743   1.98269  10.33556  10.65116
Alpha virt. eigenvalues --   10.69451  10.77105  10.83726  10.85387  10.85642
Alpha virt. eigenvalues --   10.86194  10.97373  11.12170  11.13237  11.28570
Alpha virt. eigenvalues --   11.52369  11.63720  11.63795  11.72445  11.73917
Alpha virt. eigenvalues --   11.75264  11.76659  11.78182  15.18363  15.29641
Alpha virt. eigenvalues --   15.31508  15.35644
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
    1  N    7.111907   0.385065  -0.067866  -0.008985  -0.002619   0.000104
    2  C    0.385065   4.646652   0.374441  -0.035912  -0.006196   0.000464
    3  C   -0.067866   0.374441   5.510759   0.346748  -0.076054  -0.014013
    4  C   -0.008985  -0.035912   0.346748   4.806538   0.553276  -0.153708
    5  N   -0.002619  -0.006196  -0.076054   0.553276   6.741469   0.553276
    6  C    0.000104   0.000464  -0.014013  -0.153708   0.553276   4.806538
    7  C    0.000040  -0.000177  -0.002295  -0.014013  -0.076054   0.346748
    8  C    0.000041  -0.000020  -0.000177   0.000464  -0.006196  -0.035912
    9  N   -0.000947   0.000041   0.000040   0.000104  -0.002619  -0.008985
   10  C    0.000041  -0.000006  -0.000011  -0.000007   0.002819   0.000942
   11  C    0.000040  -0.000011   0.000005  -0.000012  -0.000172  -0.000214
```

12	C	0.000104	-0.000007	-0.000012	-0.000001	0.000039	0.000003
13	N	-0.002619	0.002819	-0.000172	0.000039	-0.000246	0.000039
14	C	-0.008985	0.000942	-0.000214	0.000003	0.000039	-0.000001
15	C	-0.067866	-0.015464	-0.001652	-0.000214	-0.000172	-0.000012
16	C	0.385065	-0.095440	-0.015464	0.000942	0.002819	-0.000007
17	C	-0.107623	-0.081183	0.001819	-0.000642	-0.000050	-0.000006
18	C	-0.107623	0.462049	-0.025419	-0.003306	-0.000277	-0.000034
19	H	0.002212	-0.029820	0.003369	0.000441	-0.000001	0.000001
20	H	0.002212	0.004641	-0.000065	0.000004	0.000000	0.000000
21	H	0.002830	0.000105	0.000015	0.000000	0.000000	0.000000
22	C	0.000138	0.000054	-0.000002	0.000000	-0.000001	0.000000
23	C	-0.000071	-0.000002	0.000000	0.000000	-0.000001	0.000000
24	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
25	H	-0.000002	0.000000	0.000000	0.000000	0.000000	0.000000
26	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
27	C	0.000001	0.000000	0.000000	-0.000006	-0.000050	-0.000642
28	C	0.000001	-0.000001	-0.000002	-0.000034	-0.000277	-0.003306
29	H	0.000000	0.000000	0.000000	0.000001	-0.000001	0.000441
30	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000004
31	H	0.001612	-0.000089	-0.000130	0.000419	0.009812	0.000926
32	H	0.000000	0.000000	0.000017	-0.000009	0.001623	-0.046050
33	C	-0.000071	-0.000661	0.002621	-0.085904	-0.125475	0.384386
34	C	0.000138	0.000143	-0.036305	0.384386	-0.125475	-0.085904
35	H	-0.000002	0.000331	0.005068	-0.027032	0.003802	0.005544
36	H	0.000000	0.000002	-0.000149	0.005544	0.003802	-0.027032
37	H	0.002830	-0.047985	0.398564	-0.046050	0.001623	-0.000009
38	H	0.245460	-0.008822	-0.001813	0.000926	0.009812	0.000419

		7	8	9	10	11	12
1	N	0.000040	0.000041	-0.000947	0.000041	0.000040	0.000104
2	C	-0.000177	-0.000020	0.000041	-0.000006	-0.000011	-0.000007
3	C	-0.002295	-0.000177	0.000040	-0.000011	0.000005	-0.000012
4	C	-0.014013	0.000464	0.000104	-0.000007	-0.000012	-0.000001
5	N	-0.076054	-0.006196	-0.002619	0.002819	-0.000172	0.000039
6	C	0.346748	-0.035912	-0.008985	0.000942	-0.000214	0.000003
7	C	5.510759	0.374441	-0.067866	-0.015464	-0.001652	-0.000214
8	C	0.374441	4.646652	0.385065	-0.095440	-0.015464	0.000942
9	N	-0.067866	0.385065	7.111907	0.385065	-0.067866	-0.008985
10	C	-0.015464	-0.095440	0.385065	4.646652	0.374441	-0.035912
11	C	-0.001652	-0.015464	-0.067866	0.374441	5.510759	0.346748
12	C	-0.000214	0.000942	-0.008985	-0.035912	0.346748	4.806538
13	N	-0.000172	0.002819	-0.002619	-0.006196	-0.076054	0.553276
14	C	-0.000012	-0.000007	0.000104	0.000464	-0.014013	-0.153708
15	C	0.000005	-0.000011	0.000040	-0.000177	-0.002295	-0.014013
16	C	-0.000011	-0.000006	0.000041	-0.000020	-0.000177	0.000464
17	C	0.000000	0.000000	0.000001	-0.000001	-0.000002	-0.000034
18	C	-0.000002	-0.000001	0.000001	0.000000	0.000000	-0.000006
19	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
20	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000001
21	H	0.000000	0.000000	0.000000	0.000000	0.000017	-0.000009

22	C	0.000000	-0.000002	-0.000071	-0.000661	0.002621	-0.085904
23	C	-0.000002	0.000054	0.000138	0.000143	-0.036305	0.384386
24	H	0.000000	0.000000	-0.000002	0.000331	0.005068	-0.027032
25	H	0.000000	0.000000	0.000000	0.000002	-0.000149	0.005544
26	H	0.000015	0.000105	0.002830	-0.047985	0.398564	-0.046050
27	C	0.001819	-0.081183	-0.107623	0.462049	-0.025419	-0.003306
28	C	-0.025419	0.462049	-0.107623	-0.081183	0.001819	-0.000642
29	H	0.003369	-0.029820	0.002212	0.004641	-0.000065	0.000004
30	H	-0.000065	0.004641	0.002212	-0.029820	0.003369	0.000441
31	H	-0.001813	-0.008822	0.245460	-0.008822	-0.001813	0.000926
32	H	0.398564	-0.047985	0.002830	0.000105	0.000015	0.000000
33	C	-0.036305	0.000143	0.000138	0.000054	-0.000002	0.000000
34	C	0.002621	-0.000661	-0.000071	-0.000002	0.000000	0.000000
35	H	-0.000149	0.000002	0.000000	0.000000	0.000000	0.000000
36	H	0.005068	0.000331	-0.000002	0.000000	0.000000	0.000000
37	H	0.000017	0.000000	0.000000	0.000000	0.000000	0.000000
38	H	-0.000130	-0.000089	0.001612	-0.000089	-0.000130	0.000419
		13	14	15	16	17	18
1	N	-0.002619	-0.008985	-0.067866	0.385065	-0.107623	-0.107623
2	C	0.002819	0.000942	-0.015464	-0.095440	-0.081183	0.462049
3	C	-0.000172	-0.000214	-0.001652	-0.015464	0.001819	-0.025419
4	C	0.000039	0.000003	-0.000214	0.000942	-0.000642	-0.003306
5	N	-0.000246	0.000039	-0.000172	0.002819	-0.000050	-0.000277
6	C	0.000039	-0.000001	-0.000012	-0.000007	-0.000006	-0.000034
7	C	-0.000172	-0.000012	0.000005	-0.000011	0.000000	-0.000002
8	C	0.002819	-0.000007	-0.000011	-0.000006	0.000000	-0.000001
9	N	-0.002619	0.000104	0.000040	0.000041	0.000001	0.000001
10	C	-0.006196	0.000464	-0.000177	-0.000020	-0.000001	0.000000
11	C	-0.076054	-0.014013	-0.002295	-0.000177	-0.000002	0.000000
12	C	0.553276	-0.153708	-0.014013	0.000464	-0.000034	-0.000006
13	N	6.741469	0.553276	-0.076054	-0.006196	-0.000277	-0.000050
14	C	0.553276	4.806538	0.346748	-0.035912	-0.003306	-0.000642
15	C	-0.076054	0.346748	5.510759	0.374441	-0.025419	0.001819
16	C	-0.006196	-0.035912	0.374441	4.646652	0.462049	-0.081183
17	C	-0.000277	-0.003306	-0.025419	0.462049	5.199319	0.523088
18	C	-0.000050	-0.000642	0.001819	-0.081183	0.523088	5.199319
19	H	0.000000	0.000004	-0.000065	0.004641	-0.024568	0.366664
20	H	-0.000001	0.000441	0.003369	-0.029820	0.366664	-0.024568
21	H	0.001623	-0.046050	0.398564	-0.047985	0.000568	0.000492
22	C	-0.125475	0.384386	-0.036305	0.000143	-0.000582	0.000011
23	C	-0.125475	-0.085904	0.002621	-0.000661	0.000032	-0.000001
24	H	0.003802	0.005544	-0.000149	0.000002	0.000000	0.000000
25	H	0.003802	-0.027032	0.005068	0.000331	0.000019	0.000000
26	H	0.001623	-0.000009	0.000017	0.000000	0.000000	0.000000
27	C	-0.000277	-0.000034	-0.000002	-0.000001	0.000000	0.000000
28	C	-0.000050	-0.000006	0.000000	0.000000	0.000000	0.000000
29	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
30	H	-0.000001	0.000001	0.000000	0.000000	0.000000	0.000000
31	H	0.009812	0.000419	-0.000130	-0.000089	-0.000001	-0.000001

32	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
33	C	-0.000001	0.000000	0.000000	-0.000002	-0.000001	0.000032
34	C	-0.000001	0.000000	-0.000002	0.000054	0.000011	-0.000582
35	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000019
36	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
37	H	0.000000	0.000000	0.000015	0.000105	0.000492	0.000568
38	H	0.009812	0.000926	-0.001813	-0.008822	0.003353	0.003353
		19	20	21	22	23	24
1	N	0.002212	0.002212	0.002830	0.000138	-0.000071	0.000000
2	C	-0.029820	0.004641	0.000105	0.000054	-0.000002	0.000000
3	C	0.003369	-0.000065	0.000015	-0.000002	0.000000	0.000000
4	C	0.000441	0.000004	0.000000	0.000000	0.000000	0.000000
5	N	-0.000001	0.000000	0.000000	-0.000001	-0.000001	0.000000
6	C	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
7	C	0.000000	0.000000	0.000000	0.000000	-0.000002	0.000000
8	C	0.000000	0.000000	0.000000	-0.000002	0.000054	0.000000
9	N	0.000000	0.000000	0.000000	-0.000071	0.000138	-0.000002
10	C	0.000000	0.000000	0.000000	-0.000661	0.000143	0.000331
11	C	0.000000	0.000000	0.000017	0.002621	-0.036305	0.005068
12	C	0.000000	0.000001	-0.000009	-0.085904	0.384386	-0.027032
13	N	0.000000	-0.000001	0.001623	-0.125475	-0.125475	0.003802
14	C	0.000004	0.000441	-0.046050	0.384386	-0.085904	0.005544
15	C	-0.000065	0.003369	0.398564	-0.036305	0.002621	-0.000149
16	C	0.004641	-0.029820	-0.047985	0.000143	-0.000661	0.000002
17	C	-0.024568	0.366664	0.000568	-0.000582	0.000032	0.000000
18	C	0.366664	-0.024568	0.000492	0.000011	-0.000001	0.000000
19	H	0.453756	-0.000956	-0.000001	0.000000	0.000000	0.000000
20	H	-0.000956	0.453756	-0.000837	0.000012	0.000000	0.000000
21	H	-0.000001	-0.000837	0.487469	0.001623	0.000880	0.000000
22	C	0.000000	0.000012	0.001623	5.302294	0.535512	-0.022226
23	C	0.000000	0.000000	0.000880	0.535512	5.302294	0.349448
24	H	0.000000	0.000000	0.000000	-0.022226	0.349448	0.468300
25	H	0.000000	0.000000	-0.001186	0.349448	-0.022226	0.000348
26	H	0.000000	0.000000	0.000000	0.000880	0.001623	-0.001186
27	C	0.000000	0.000000	0.000000	0.000032	-0.000582	0.000019
28	C	0.000000	0.000000	0.000000	-0.000001	0.000011	0.000000
29	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
30	H	0.000000	0.000000	0.000000	0.000000	0.000012	0.000000
31	H	0.000000	0.000000	0.000000	0.000079	0.000046	-0.000001
32	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
33	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
34	C	0.000012	0.000000	0.000000	0.000000	0.000000	0.000000
35	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
36	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
37	H	-0.000837	-0.000001	0.000000	0.000000	0.000000	0.000000
38	H	-0.000033	-0.000033	0.000028	0.000046	0.000079	0.000000
		25	26	27	28	29	30
1	N	-0.000002	0.000000	0.000001	0.000001	0.000000	0.000000
2	C	0.000000	0.000000	0.000000	-0.000001	0.000000	0.000000

3	C	0.000000	0.000000	0.000000	-0.000002	0.000000	0.000000
4	C	0.000000	0.000000	-0.000006	-0.000034	0.000001	0.000000
5	N	0.000000	0.000000	-0.000050	-0.000277	-0.000001	0.000000
6	C	0.000000	0.000000	-0.000642	-0.003306	0.000441	0.000004
7	C	0.000000	0.000015	0.001819	-0.025419	0.003369	-0.000065
8	C	0.000000	0.000105	-0.081183	0.462049	-0.029820	0.004641
9	N	0.000000	0.002830	-0.107623	-0.107623	0.002212	0.002212
10	C	0.000002	-0.047985	0.462049	-0.081183	0.004641	-0.029820
11	C	-0.000149	0.398564	-0.025419	0.001819	-0.000065	0.003369
12	C	0.005544	-0.046050	-0.003306	-0.000642	0.000004	0.000441
13	N	0.003802	0.001623	-0.000277	-0.000050	0.000000	-0.000001
14	C	-0.027032	-0.000009	-0.000034	-0.000006	0.000000	0.000001
15	C	0.005068	0.000017	-0.000002	0.000000	0.000000	0.000000
16	C	0.000331	0.000000	-0.000001	0.000000	0.000000	0.000000
17	C	0.000019	0.000000	0.000000	0.000000	0.000000	0.000000
18	C	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
19	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
20	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
21	H	-0.001186	0.000000	0.000000	0.000000	0.000000	0.000000
22	C	0.349448	0.000880	0.000032	-0.000001	0.000000	0.000000
23	C	-0.022226	0.001623	-0.000582	0.000011	0.000000	0.000012
24	H	0.000348	-0.001186	0.000019	0.000000	0.000000	0.000000
25	H	0.468300	0.000000	0.000000	0.000000	0.000000	0.000000
26	H	0.000000	0.487469	0.000568	0.000492	-0.000001	-0.000837
27	C	0.000000	0.000568	5.199319	0.523088	-0.024568	0.366664
28	C	0.000000	0.000492	0.523088	5.199319	0.366664	-0.024568
29	H	0.000000	-0.000001	-0.024568	0.366664	0.453756	-0.000956
30	H	0.000000	-0.000837	0.366664	-0.024568	-0.000956	0.453756
31	H	0.000000	0.000028	0.003353	0.003353	-0.000033	-0.000033
32	H	0.000000	0.000000	0.000492	0.000568	-0.000837	-0.000001
33	C	0.000000	0.000000	0.000011	-0.000582	0.000012	0.000000
34	C	0.000000	0.000000	-0.000001	0.000032	0.000000	0.000000
35	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
36	H	0.000000	0.000000	0.000000	0.000019	0.000000	0.000000
37	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
38	H	-0.000001	0.000000	-0.000001	-0.000001	0.000000	0.000000
		31	32	33	34	35	36
1	N	0.001612	0.000000	-0.000071	0.000138	-0.000002	0.000000
2	C	-0.000089	0.000000	-0.000661	0.000143	0.000331	0.000002
3	C	-0.000130	0.000017	0.002621	-0.036305	0.005068	-0.000149
4	C	0.000419	-0.000009	-0.085904	0.384386	-0.027032	0.005544
5	N	0.009812	0.001623	-0.125475	-0.125475	0.003802	0.003802
6	C	0.000926	-0.046050	0.384386	-0.085904	0.005544	-0.027032
7	C	-0.001813	0.398564	-0.036305	0.002621	-0.000149	0.005068
8	C	-0.008822	-0.047985	0.000143	-0.000661	0.000002	0.000331
9	N	0.245460	0.002830	0.000138	-0.000071	0.000000	-0.000002
10	C	-0.008822	0.000105	0.000054	-0.000002	0.000000	0.000000
11	C	-0.001813	0.000015	-0.000002	0.000000	0.000000	0.000000
12	C	0.000926	0.000000	0.000000	0.000000	0.000000	0.000000

13	N	0.009812	0.000000	-0.000001	-0.000001	0.000000	0.000000
14	C	0.000419	0.000000	0.000000	0.000000	0.000000	0.000000
15	C	-0.000130	0.000000	0.000000	-0.000002	0.000000	0.000000
16	C	-0.000089	0.000000	-0.000002	0.000054	0.000000	0.000000
17	C	-0.000001	0.000000	-0.000001	0.000011	0.000000	0.000000
18	C	-0.000001	0.000000	0.000032	-0.000582	0.000019	0.000000
19	H	0.000000	0.000000	0.000000	0.000012	0.000000	0.000000
20	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
21	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
22	C	0.000079	0.000000	0.000000	0.000000	0.000000	0.000000
23	C	0.000046	0.000000	0.000000	0.000000	0.000000	0.000000
24	H	-0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
25	H	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
26	H	0.000028	0.000000	0.000000	0.000000	0.000000	0.000000
27	C	0.003353	0.000492	0.000011	-0.000001	0.000000	0.000000
28	C	0.003353	0.000568	-0.000582	0.000032	0.000000	0.000019
29	H	-0.000033	-0.000837	0.000012	0.000000	0.000000	0.000000
30	H	-0.000033	-0.000001	0.000000	0.000000	0.000000	0.000000
31	H	0.202974	0.000028	0.000046	0.000079	0.000000	-0.000001
32	H	0.000028	0.487469	0.001623	0.000880	0.000000	-0.001186
33	C	0.000046	0.001623	5.302294	0.535512	-0.022226	0.349448
34	C	0.000079	0.000880	0.535512	5.302294	0.349448	-0.022226
35	H	0.000000	0.000000	-0.022226	0.349448	0.468300	0.000348
36	H	-0.000001	-0.001186	0.349448	-0.022226	0.000348	0.468300
37	H	0.000000	0.000000	0.000880	0.001623	-0.001186	0.000000
38	H	0.002360	0.000000	0.000079	0.000046	-0.000001	0.000000

		37	38
1	N	0.002830	0.245460
2	C	-0.047985	-0.008822
3	C	0.398564	-0.001813
4	C	-0.046050	0.000926
5	N	0.001623	0.009812
6	C	-0.000009	0.000419
7	C	0.000017	-0.000130
8	C	0.000000	-0.000089
9	N	0.000000	0.001612
10	C	0.000000	-0.000089
11	C	0.000000	-0.000130
12	C	0.000000	0.000419
13	N	0.000000	0.009812
14	C	0.000000	0.000926
15	C	0.000015	-0.001813
16	C	0.000105	-0.008822
17	C	0.000492	0.003353
18	C	0.000568	0.003353
19	H	-0.000837	-0.000033
20	H	-0.000001	-0.000033
21	H	0.000000	0.000028
22	C	0.000000	0.000046

23	C	0.000000	0.000079
24	H	0.000000	0.000000
25	H	0.000000	-0.000001
26	H	0.000000	0.000000
27	C	0.000000	-0.000001
28	C	0.000000	-0.000001
29	H	0.000000	0.000000
30	H	0.000000	0.000000
31	H	0.000000	0.002360
32	H	0.000000	0.000000
33	C	0.000880	0.000079
34	C	0.001623	0.000046
35	H	-0.001186	-0.000001
36	H	0.000000	0.000000
37	H	0.487469	0.000028
38	H	0.000028	0.202974

Mulliken atomic charges:

		1
1	N	-0.764562
2	C	0.444045
3	C	-0.401650
4	C	0.276000
5	N	-0.462272
6	C	0.276000
7	C	-0.401650
8	C	0.444045
9	N	-0.764562
10	C	0.444045
11	C	-0.401650
12	C	0.276000
13	N	-0.462272
14	C	0.276000
15	C	-0.401650
16	C	0.444045
17	C	-0.313720
18	C	-0.313720
19	H	0.225181
20	H	0.225181
21	H	0.201856
22	C	-0.306051
23	C	-0.306051
24	H	0.217735
25	H	0.217735
26	H	0.201856
27	C	-0.313720
28	C	-0.313720
29	H	0.225181
30	H	0.225181
31	H	0.540043

```
   32  H    0.201856
   33  C   -0.306051
   34  C   -0.306051
   35  H    0.217735
   36  H    0.217735
   37  H    0.201856
   38  H    0.540043
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  N   -0.224519
    2  C    0.444045
    3  C   -0.199794
    4  C    0.276000
    5  N   -0.462272
    6  C    0.276000
    7  C   -0.199794
    8  C    0.444045
    9  N   -0.224519
   10  C    0.444045
   11  C   -0.199794
   12  C    0.276000
   13  N   -0.462272
   14  C    0.276000
   15  C   -0.199794
   16  C    0.444045
   17  C   -0.088540
   18  C   -0.088540
   19  H    0.000000
   20  H    0.000000
   21  H    0.000000
   22  C   -0.088316
   23  C   -0.088316
   24  H    0.000000
   25  H    0.000000
   26  H    0.000000
   27  C   -0.088540
   28  C   -0.088540
   29  H    0.000000
   30  H    0.000000
   31  H    0.000000
   32  H    0.000000
   33  C   -0.088316
   34  C   -0.088316
   35  H    0.000000
   36  H    0.000000
   37  H    0.000000
   38  H    0.000000
Sum of Mulliken charges=   0.00000
```

```
Electronic spatial extent (au):  <R**2>=  7683.8276
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     0.0000    Y=     0.0000    Z=     0.0000  Tot=     0.0000
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=  -154.7557   YY=  -117.2677   ZZ=  -107.1650
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=   -28.3596   YY=     9.1285   ZZ=    19.2312
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=     0.0000  YYY=     0.0000  ZZZ=     0.0000  XYY=     0.0000
 XXY=     0.0000  XXZ=     0.0000  XZZ=     0.0000  YZZ=     0.0000
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=  -182.0508 YYYY= -4819.9941 ZZZZ= -4653.8027 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY= -1062.3973 XXZZ= -1064.4300 YYZZ= -1512.0636
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 1.847455698009D+03 E-N=-5.986066886369D+03  KE= 9.819911244482D+02
Symmetry AG   KE= 2.884197450548D+02
Symmetry B1G  KE= 6.700318884468D+00
Symmetry B2G  KE= 6.998072363256D+00
Symmetry B3G  KE= 1.875664889780D+02
Symmetry AU   KE= 4.335606164032D+00
Symmetry B1U  KE= 2.378452044070D+02
Symmetry B2U  KE= 2.382526639122D+02
Symmetry B3U  KE= 1.187302468450D+01

Test job not archived.
1¥1¥GINC-MIRAI86¥SP¥RSACCI¥Gen¥C20H14N4¥MASAHIRO¥31-Jul-2004¥0¥¥# SAC-
CI(SINGLET=(NSTATE=(0,0,0,0,0,4,4,1)), LEVELONE,WINDOW=(25,244))/GEN T
EST¥¥Gaussian Test Job 637: SAC-CI SD-R LevelOne calculation of optica
lly-allowed singlet excited states of Free-Base Porphin using Huzinaga
 basis sets [4s2p/2s]. Inner-shells are excluded from the active space
 and full-valence active MOs are used (FC; default): 57 occupied and 1
63 unoccupied MOs are included in the active space of SAC-CI. CPU memo
ry of 700MB is specified with %mem to allocate electron repulsion inte
grals in core memory (all ERIs are stored on cpu). If the core memory
is not enough for allocating all the repulsion integrals, according to
 the available memory, the program will automatically divide the integ
ral file into appropriate number of files which are sequentially alloc
ated on the core memory. Experimental results and the results of Level
Two calculations are compared in Pa¥¥0,1¥N,0,2.122283,0.,0.¥C,0,2.9039
91,1.131654,0.¥C,0,2.43106,2.448915,0.¥C,0,1.087013,2.860819,0.¥N,0,0.
,2.032117,0.¥C,0,-1.087013,2.860819,0.¥C,0,-2.43106,2.448915,0.¥C,0,-2
.903991,1.131654,0.¥N,0,-2.122283,0.,0.¥C,0,-2.903991,-1.131654,0.¥C,0
,-2.43106,-2.448915,0.¥C,0,-1.087013,-2.860819,0.¥N,0,0.,-2.032117,0.¥
C,0,1.087013,-2.860819,0.¥C,0,2.43106,-2.448915,0.¥C,0,2.903991,-1.131
```

```
654,0.¥C,0,4.274858,-0.690194,0.¥C,0,4.274858,0.690194,0.¥H,0,5.131714
,1.353489,0.¥H,0,5.131714,-1.353489,0.¥H,0,3.188699,-3.229008,0.¥C,0,0
.682348,-4.268828,0.¥C,0,-0.682348,-4.268828,0.¥H,0,-1.357121,-5.11833
7,0.¥H,0,1.357121,-5.118337,0.¥H,0,-3.188699,-3.229008,0.¥C,0,-4.27485
8,-0.690194,0.¥C,0,-4.274858,0.690194,0.¥H,0,-5.131714,1.353489,0.¥H,0
,-5.131714,-1.353489,0.¥H,0,-1.106269,0.,0.¥H,0,-3.188699,3.229008,0.¥
C,0,-0.682348,4.268828,0.¥C,0,0.682348,4.268828,0.¥H,0,1.357121,5.1183
37,0.¥H,0,-1.357121,5.118337,0.¥H,0,3.188699,3.229008,0.¥H,0,1.106269,
0.,0.¥¥Version=AI64T-G03RevC.02¥State=1-AG¥HF=-982.9254061¥RMSD=7.737e
-09¥PG=DO2H [C2'(N1.N1),C2"(N1H1.H1N1),SG(C2OH12)]¥¥@


HE THAT WALD REACHE THE SWEITE ROSE
SULD NOW AND THEN BE SCRATCHED WT THE SCHARPE BREERES.
-- PROVERBS AND REASONS OF THE YEAR 1585
          AS REPRINTED IN PAISLEY MAGAZINE 1828.
Job cpu time:  0 days  2 hours 38 minutes 15.6 seconds.
File lengths (MBytes):  RWF=   8138 Int=      0 D2E=      0 Chk=     46 Scr=   1363
Normal termination of Gaussian 03 at Sat Jul 31 15:24:02 2004.
```

Output 638

```
Entering Gaussian System, Link 0=/work/g03.C02/g03/g03
Initial command:
/work/g03.C02/g03/l1.exe /work/g03.C02/inputs/Gau-184914.inp -scrdir=/work/g03.C02/inputs/
Entering Link 1 = /work/g03.C02/g03/l1.exe PID=    184915.

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M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,
A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

```
*****************************************
Gaussian 03:  AI64T-G03RevC.02 12-Jun-2004
                 3-Aug-2004
*****************************************
%mem=12mw
---------------------------------------------------------------------------
# SAC-CI(Singlet=(NState=(0,1)), TargetState=(SpinState=Singlet,Symmet
ry=2,Root=1)) /D95(d) Opt test
---------------------------------------------------------------------------
1/18=20,38=1/1,3;
2/9=110,17=6,18=5,40=1/2;
3/5=8,7=1,11=9,16=1,25=1,30=1,36=2/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=5,9=30000,10=1,40=1,41=2,42=2/1,4;
9/15=1/23;
11/28=-13,29=200,42=3,46=2/11;
10/5=5/2;
6/7=2,8=2,9=2,10=2/1;
7/12=7/1,2,3,16;
1/18=20/3(1);
99//99;
2/9=110/2;
3/5=8,7=1,11=9,16=1,25=1,30=1,36=2/1,2,3;
4/5=5,16=3/1;
5/5=2,38=5/2;
8/6=5,9=30000,10=1,40=1,41=2,42=2/1,4;
9/15=1/23;
11/28=-13,29=200,42=3,46=2/11;
10/5=5/2;
7/12=7/1,2,3,16;
1/18=20/3(-9);
2/9=110/2;
6/7=2,8=2,9=2,10=2/1;
99//99;
---------------------------------------------------------------------------
Gaussian Test Job 638 (Part 1): SAC-CI SD-R geometry optimization for
the singlet ground (A') and A" excited state of HCF with D95(d) basis.
 Minimum-Orbital Deformation (MOD) method is used and full-valence act
ive MOs are adopted (FC; default). First is the geometry optimization
for the excited A" state. Initial geometry is the experimental one. Th
e results are compared with experiments in Part I-L of the SAC-CI Guid
e.
---------------------------------------------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C
F                    1    FC
H                    1    HC       2    HCF
```

List of keywords given in the Gaussian input. This input calculates geometry of the first-excited state in singlet A" symmetry.

Brief description of the current test job.

Nuclear coordinates for HCF given in the Gaussian input

```
     Variables:
 FC                    1.308
 HC                    1.063
 HCF                  123.8


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                          ----------------------------
                          !    Initial Parameters    !
                          ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                   1.308          estimate D2E/DX2                !
! R2    R(1,3)                   1.063          estimate D2E/DX2                !
! A1    A(2,1,3)               123.8            estimate D2E/DX2                !
--------------------------------------------------------------------------------
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6          0        0.000000    0.000000    0.000000
   2          9          0        0.000000    0.000000    1.308000
   3          1          0        0.883336    0.000000   -0.591342
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3
    1  C    0.000000
    2  F    1.308000   0.000000
    3  H    1.063000   2.094704   0.000000
Stoichiometry    CHF
Framework group  CS[SG(CHF)]
Deg. of freedom     3
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6          0        0.055209    0.698791    0.000000
```

Nuclear coordinates used in the actual calculation

```
   2          9             0        0.055209   -0.609209    0.000000
   3          1             0       -0.828128    1.290133    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    768.9389466     34.6597728     33.1648726
Standard basis: D95(d) (6D, 7F)
There are    26 symmetry adapted basis functions of A'  symmetry.
There are     8 symmetry adapted basis functions of A"  symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   34 basis functions,    64 primitive gaussians,    34 cartesian basis functions
    8 alpha electrons        8 beta electrons
      nuclear repulsion energy        27.1072910664 Hartrees.
NAtoms=    3 NActive=    3 NUniq=    3 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    34 RedAO= T  NBF=    26     8
NBsUse=    34 1.00D-06 NBFU=    26     8
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.15D-01 ExpMax= 9.99D+03 ExpMxC= 1.51D+03 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=         1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Initial guess orbital symmetries:
      Occupied  (A') (A') (A') (A') (A') (A") (A') (A')
      Virtual   (A") (A') (A') (A') (A") (A') (A') (A') (A") (A')
                (A') (A') (A") (A") (A') (A') (A') (A") (A') (A")
                (A') (A') (A') (A') (A') (A')
The electronic state of the initial guess is 1-A'.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=     1040327.
SCF Done:  E(RHF) =  -137.771435792     A.U. after   12 cycles
            Convg  =    0.4133D-08             -V/T =  2.0002
            S**2   =   0.0000
ExpMin= 1.15D-01 ExpMax= 9.99D+03 ExpMxC= 1.51D+03 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=         1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     3    32
Use canonical orbitals as reference of MOD.
  Overlap analysis:     1 - Trace/N =  0.000000
                   Max |<i|i> - 1| =  0.000000
                   Max  <i|j>      =  0.000000
                   Min eigenvalue  =  1.000000
  Overlap analysis:     1 - Trace/N =  0.000000
                   Max |<i|i> - 1| =  0.000000
                   Max  <i|j>      =  0.000000
                   Min eigenvalue  =  1.000000
NBasis=    34 NAE=     8 NBE=     8 NFC=     2 NFV=     2
```

Hartree-Fock SCF energy at the initial geometry.

AO to MO transformation of two-electron repulsion integrals

```
NROrb=     30 NOA=     6 NOB=     6 NVA=    24 NVB=    24
-----------------------------------------------------------------------
#######################################################################
-----------------------------------------------------------------------
              SAC/SAC-CI Program Combined with GAUSSIAN
                              for Calculating
        Ground, Excited, Ionized, and Electron-Attached States
                                 and
             Singlet, Doublet, Triplet, Quartet, Quintet,
                   Sextet, and Septet Spin States
                                 and
                  Their Analytical Energy Gradients
                         coded originally by
                          Hiroshi Nakatsuji
                           and extended by
 H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa,
       M. Ishida, T. Nakajima, Y. Honda, O. Kitao, and H. Nakai
                                 at
                 Department of Hydrocarbon Chemistry,
                Division of Molecular Engineering, and
      Department of Synthetic Chemistry & Biological Chemistry,
                  Graduate School of Engineering,
                          Kyoto University,
                        Kyoto 606-8501, Japan
-----------------------------------------------------------------------
#######################################################################
-----------------------------------------------------------------------
No. of INTEGRALS =     57481 NBLK =        35 KOUNT =      1481
*******************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 0
*******************************************************************************
================================================================
  STEP #PRES#  Generation of Linked Operators and Selection
================================================================
== States to be calculated ==
           AG   AU
SINGLET    Yes  Yes
TRIPLET    No   No
IONIZED    No   No
ANIONIZED  No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  1)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
****************************
        SINGLET STATE
****************************
```

Beginning of the SAC-CI part of the program

```
-----------------------------------------------------------------
LINKED OPERATORS FOR SAC:    SYMMETRY = A'  GROUND STATE
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            92        5656         5748
    AFTER             92        4176         4269
-----------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = A'' EXCITED STATE
  #SECI# Main reference configuration and coefficient
    ##   1-st state ##       energy (au) =       0.060668
       8 ->   9     0.97259        8 ->  13    -0.21740
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            52        4784         4836
    AFTER             52        2000         2052
=================================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
=================================================================
=================================================================
  STEP #DIAGCI#  Solution of SDCI
=================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A'    CONVERGED
Solution for Singlet   A''   CONVERGED
=================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
=================================================================
Threshold for S2 operator (CThreULS2G) 0.500D-02
=================================================================
  STEP #SAC#  Solution of SAC equation
=================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*****************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*****************************************
HF ENERGY     =    -137.771436 (AU)
SAC-NV  ENERGY=      -0.277684 (AU)
TOTAL ENERGY  =    -138.049120 (AU)
=====================================================================
  STEP #ULINTS#  Unlinked integral for Singlet Excited State (SAC-CI)
=====================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
=================================================================
```

Number of the linked operators for single- and double- excitation operators before and after the perturbation selection

Main configurations of the reference SECI calculation used for the perturbation selection step. For example, the first excited state in singlet A" symmetry is the transition from 8-th MO to 9-th MO, and its CI coefficient is about 0.97.

Result of SAC calculation. Hartree-Fock (HF) energy, SAC-NV energy (correlation energy obtained with the SAC method).

```
  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
================================================================
Threshold for density convergence (DConvDiag) .100D-
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A''   CONVERGED
**********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
**********************************************
*****************************************************
Singlet       A''     *****************************************************
###   1-st  ###          ---   1st state in this spin multiplicity ---
    This state is being used for optimizations.
    Total energy       in au =    -137.983401
    Correlation energy in au =      -0.211965
    Excitation energy  in au =       0.065719    in eV =       1.788293
  *SINGLE EXCITATION
       8    9     0.95979         8   13    -0.20816
       7    9    -0.04960         4    9    -0.03233
  *DOUBLE EXCITATION
       8   23    8    9     0.06174         8   13    8   12    -0.05303
       8   14    8   13    -0.03808         6    9    5    9     0.03703
       8   23    4    9     0.03604         8    9    6    9     0.03352
================================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
================================================================
Energy gradient for SINGLET STATE A''  1-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-CI-V)=   -0.2119653410 Total energy=      -137.9834011329
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-CI-V / SAC-NV density.
Gamma from SAC-CI-V (singlet). Symmetry  2
Start back-transformation.
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     595
Number of TU pair in the last loop  =     595
Second-half back-transformation finished.
Solve CP equations for MOD among active MOs.
Max orbital gradient: YijMax=  0.001520 YabMax=  0.003120
DoAtom=TTT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      997720.
```

Result of SAC-CI calculation. Total energy, correlation energy (HF energy as the reference), excitation energy (SAC total energy as the reference), and the SAC-CI coefficients are shown. For example, the first excited state in singlet A" symmetry is the excitation from 8-th MO to 9-th MO, and its excitation energy is 1.79 eV.

Solving Z-vector equation for the target state.

```
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
    1 vectors were produced by pass  8.
    1 vectors were produced by pass  9.
    1 vectors were produced by pass 10.
    1 vectors were produced by pass 11.
Inv2:  IOpt= 1 Iter= 1 AM= 4.49D-16 Conv= 1.00D-12.
Inverted reduced A of dimension   12 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.

******************************************************************

           Population analysis using the SCF density.

******************************************************************

Orbital symmetries:
      Occupied  (A') (A') (A') (A') (A') (A″) (A') (A')
      Virtual   (A″) (A') (A') (A') (A″) (A') (A') (A') (A″) (A')
                (A') (A') (A″) (A″) (A') (A') (A') (A″) (A') (A″)
                (A') (A') (A') (A') (A') (A')
The electronic state is 1-A'.
Alpha  occ. eigenvalues --  -26.35847 -11.36075  -1.67788  -0.92642  -0.76890
Alpha  occ. eigenvalues --   -0.71443  -0.70419  -0.37409
Alpha virt. eigenvalues --    0.07188   0.25131   0.36827   0.42100   0.49409
Alpha virt. eigenvalues --    0.59546   0.68126   1.00911   1.11311   1.16814
Alpha virt. eigenvalues --    1.24533   1.41605   1.73779   1.77975   1.78880
Alpha virt. eigenvalues --    2.11485   2.27765   2.36204   2.41027   2.84705
Alpha virt. eigenvalues --    2.95364   3.20941   4.04369   4.37271  27.39023
Alpha virt. eigenvalues --   56.51137
         Condensed to atoms (all electrons):
             1          2          3
    1  C    5.518680   0.219759   0.239722
    2  F    0.219759   8.994027  -0.020415
    3  H    0.239722  -0.020415   0.609163
Mulliken atomic charges:
             1
    1  C    0.021839
    2  F   -0.193370
    3  H    0.171531
Sum of Mulliken charges=   0.00000
```

```
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  C    0.193370
    2  F   -0.193370
    3  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    56.1948
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=    -1.9752    Y=     0.4154    Z=     0.0000  Tot=     2.0184
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=   -12.2238   YY=   -11.7590   ZZ=    -9.9764
  XY=    -2.4314   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -0.9041   YY=    -0.4393   ZZ=     1.3433
  XY=    -2.4314   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=    -2.1385  YYY=    -6.7705  ZZZ=     0.0000  XYY=    -3.3315
 XXY=    -3.1430  XXZ=     0.0000  XZZ=    -0.5962  YZZ=    -1.5159
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=   -15.3987 YYYY=   -43.8399 ZZZZ=    -7.4060 XXXY=    -0.6004
XXXZ=     0.0000 YYYX=    -3.2017 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=   -10.6749 XXZZ=    -3.8509 YYZZ=    -8.4109
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=    -0.0163
N-N= 2.710729106638D+01 E-N=-3.817305555966D+02  KE= 1.377433864606D+02
Symmetry A'   KE= 1.318340147902D+02
Symmetry A"   KE= 5.909371670338D+00
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6          -0.023085254    0.000000000    0.011996360
   2          9          -0.000052346    0.000000000    0.004401896
   3          1           0.023137599    0.000000000   -0.016398256
-------------------------------------------------------------------
Cartesian Forces:  Max     0.023137599 RMS     0.012911977

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.028459702 RMS     0.016627520
Search for a local minimum.
Step number   1 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- first step.
The second derivative matrix:
                          R1        R2        A1
          R1           0.65019
```

Energy gradient in cartesian coordinate calculated at the initial geometry.

```
          R2           0.00000   0.38129
          A1           0.00000   0.00000   0.16000
    Eigenvalues ---    0.16000   0.38129   0.65019
RFO step:  Lambda=-2.14625297D-03.
Linear search not attempted -- first point.
Iteration  1 RMS(Cart)=  0.03619146 RMS(Int)=  0.00017958
Iteration  2 RMS(Cart)=  0.00019383 RMS(Int)=  0.00000002
Iteration  3 RMS(Cart)=  0.00000002 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1         2.47176   0.00431   0.00000   0.00661   0.00661   2.47837
   R2         2.00878   0.02846   0.00000   0.07422   0.07422   2.08300
   A1         2.16072   0.00093   0.00000   0.00577   0.00577   2.16648
        Item               Value     Threshold  Converged?
Maximum Force            0.028460     0.000450     NO
RMS     Force            0.016628     0.000300     NO
Maximum Displacement     0.039712     0.001800     NO
RMS     Displacement     0.036268     0.001200     NO
Predicted change in Energy=-1.079121D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6           0       -0.010368    0.000000    0.008761
   2          9           0       -0.006547    0.000000    1.320254
   3          1           0        0.900251    0.000000   -0.612357
---------------------------------------------------------------------
                    Distance matrix (angstroms):
                    1          2          3
    1  C    0.000000
    2  F    1.311498   0.000000
    3  H    1.102277   2.134776   0.000000
Stoichiometry    CHF
Framework group  CS[SG(CHF)]
Deg. of freedom     3
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6           0        0.057027    0.699064    0.000000
   2          9           0        0.057027   -0.612434    0.000000
   3          1           0       -0.855398    1.317527    0.000000
```

The largest remaining force is in the R2 (H-C distance).

Energy gradient and displacements do not satisfy convergence criteria.

The second geometry to be calculated.

```
---------------------------------------------------------------------------
Rotational constants (GHZ):     724.6525458     34.2867707     32.7377896
Standard basis: D95(d) (6D, 7F)
There are    26 symmetry adapted basis functions of A'  symmetry.
There are     8 symmetry adapted basis functions of A"  symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   34 basis functions,    64 primitive gaussians,    34 cartesian basis functions
    8 alpha electrons        8 beta electrons
      nuclear repulsion energy        26.8999128264 Hartrees.
NAtoms=    3 NActive=    3 NUniq=    3 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    34 RedAO= T  NBF=    26     8
NBsUse=    34 1.00D-06 NBFU=    26     8
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A') (A') (A') (A') (A') (A") (A') (A')
      Virtual   (A") (A') (A') (A') (A") (A') (A') (A') (A") (A')
                (A') (A') (A") (A") (A') (A') (A') (A") (A') (A")
                (A') (A') (A') (A') (A') (A')
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.15D-01 ExpMax= 9.99D+03 ExpMxC= 1.51D+03 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=         1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=     1040327.
SCF Done:  E(RHF) =  -137.771551493     A.U. after   10 cycles
           Convg  =    0.9627D-08             -V/T =  2.0006
           S**2   =   0.0000
ExpMin= 1.15D-01 ExpMax= 9.99D+03 ExpMxC= 1.51D+03 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=         1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     3    32
Transform orbitals by the MOD method.
  Overlap analysis:     1 - Trace/N =  0.000671
                   Max |<i|i> - 1| =  0.003109
                   Max  <i|j>      =  0.002787
                   Min eigenvalue  =  0.996103
  Overlap analysis:     1 - Trace/N = -0.004367
                   Max |<i|i> - 1| =  0.041067
                   Max  <i|j>      =  0.021312
                   Min eigenvalue  =  0.934193
NBasis=    34 NAE=     8 NBE=     8 NFC=     2 NFV=     2
NROrb=     30 NOA=     6 NOB=     6 NVA=    24 NVB=    24
Non-canonical MOs are used.
```

MOD transformation within each occupied and virtural blocks of MOs. Checking the "displaced" overlap matrix elements. See section I-D-8 for details.

```
No. of INTEGRALS =     57481 NBLK =        35 KOUNT =      1481
*******************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 1
*******************************************************************************
================================================================
  STEP #PRES#  Generation of Linked Operators and Selection
================================================================
== States to be calculated ==
           AG   AU
SINGLET    Yes  Yes
TRIPLET    No   No
IONIZED    No   No
ANIONIZED  No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  1)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
  ---------------------------------------------------------------
   During geometry optimization, the same linked and unlinked
   operators are used.
  ---------------------------------------------------------------
****************************
        SINGLET STATE
****************************
================================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A'    CONVERGED
Solution for Singlet   A''   CONVERGED
================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
================================================================
================================================================
  STEP #SAC#  Solution of SAC equation
================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
```

By combined use of GSUM and MOD method, equivalent sets of linked and unlinked terms are used during optimization. No new perturbation selection carried out.

```
*******************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*******************************************
HF ENERGY     =    -137.771551 (AU)
SAC-NV  ENERGY=      -0.278982 (AU)
TOTAL ENERGY  =    -138.050533 (AU)
=====================================================================
  STEP #ULINTS#  Unlinked integral for Singlet Excited State (SAC-CI)
=====================================================================
================================================================
  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A''   CONVERGED
***********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
***********************************************
*****************************************************************************
Singlet       A''     ***************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    This state is being used for optimizations.
    Total energy       in au =    -137.984435
    Correlation energy in au =      -0.212884
    Excitation energy  in au =       0.066098    in eV =       1.798619
  *SINGLE EXCITATION
       8    9     0.95900         8   13    -0.20784
       7    9    -0.05642         4    9    -0.03820
  *DOUBLE EXCITATION
       8   23    8    9     0.06177         8   13    8   12    -0.05299
       8   14    8   13    -0.03804         6    9    5    9     0.03675
       8   23    4    9     0.03555         8    9    6    9     0.03306
       8   11    4    9     0.03029
================================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
================================================================
Energy gradient for SINGLET STATE A''  1-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-CI-V)=   -0.2128836403 Total energy=      -137.9844351337
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-CI-V / SAC-NV density.
Gamma from SAC-CI-V (singlet). Symmetry  2
Start back-transformation.
First-half back-transformation finished.
```

SAC-CI result at the updated geometry. The total energy is decreasing compared with that at the last geometry (-137.983401 au)

```
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     595
Number of TU pair in the last loop  =     595
Second-half back-transformation finished.
Solve CP equations for MOD among active MOs.
Max orbital gradient: YijMax=  0.002102 YabMax=  0.003146
DoAtom=TTT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      997720.
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
    1 vectors were produced by pass  8.
    1 vectors were produced by pass  9.
    1 vectors were produced by pass 10.
    1 vectors were produced by pass 11.
Inv2:  IOpt= 1 Iter= 1 AM= 3.24D-16 Conv= 1.00D-12.
Inverted reduced A of dimension   12 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6          -0.001717080    0.000000000   -0.000917897
   2          9           0.001185272    0.000000000    0.000333556
   3          1           0.000531808    0.000000000    0.000584341
-------------------------------------------------------------------
Cartesian Forces:  Max     0.001717080 RMS     0.000811809

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Berny optimization.
Internal  Forces:  Max     0.002194451 RMS     0.001281111
Search for a local minimum.
Step number   2 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using D2CorX and points  1  2
Trust test= 9.58D-01 RLast= 7.47D-02 DXMaxT set to 3.00D-01
The second derivative matrix:
                        R1        R2        A1
```

Energy gradient in cartesian coordinate calculated at the updated geometry.

```
          R1          0.64923
          R2         -0.00345   0.37866
          A1          0.00407   0.02905   0.16417
    Eigenvalues ---   0.16027   0.38249   0.64931
RFO step:  Lambda=-3.04398039D-05.
Quartic linear search produced a step of  0.00243.
Iteration  1 RMS(Cart)=  0.00842487 RMS(Int)=  0.00004384
Iteration  2 RMS(Cart)=  0.00004267 RMS(Int)=  0.00000000
Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.47837   0.00025   0.00002   0.00047   0.00048   2.47886
   R2        2.08300   0.00021   0.00018   0.00145   0.00163   2.08463
   A1        2.16648  -0.00219   0.00001  -0.01367  -0.01366   2.15282
        Item               Value     Threshold  Converged?
Maximum Force            0.002194     0.000450     NO
RMS     Force            0.001281     0.000300     NO
Maximum Displacement     0.008390     0.001800     NO
RMS     Displacement     0.008444     0.001200     NO
Predicted change in Energy=-1.522142D-05
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6           0       -0.014808    0.000000    0.006521
   2          9           0       -0.003112    0.000000    1.318223
   3          1           0        0.901256    0.000000   -0.608086
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3
    1  C    0.000000
    2  F    1.311755   0.000000
    3  H    1.103139   2.128039   0.000000
Stoichiometry    CHF
Framework group  CS[SG(CHF)]
Deg. of freedom     3
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6           0        0.057594    0.699961    0.000000
   2          9           0        0.057594   -0.611794    0.000000
```

The largest remaining force is in the A1 (H-C-F angle).

Energy gradient and displacements do not satisfy convergence criteria.

The third geometry to be calculated.

```
   3          1              0        -0.863913     1.306376     0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    708.8488652     34.3501939     32.7625495
Standard basis: D95(d) (6D, 7F)
There are    26 symmetry adapted basis functions of A'  symmetry.
There are     8 symmetry adapted basis functions of A"  symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   34 basis functions,    64 primitive gaussians,    34 cartesian basis functions
    8 alpha electrons        8 beta electrons
      nuclear repulsion energy        26.9004633008 Hartrees.
NAtoms=    3 NActive=    3 NUniq=    3 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    34 RedAO= T  NBF=    26     8
NBsUse=    34 1.00D-06 NBFU=    26     8
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A') (A') (A') (A') (A') (A") (A') (A')
      Virtual   (A") (A') (A') (A') (A") (A') (A') (A') (A") (A')
                (A') (A') (A") (A") (A') (A') (A') (A") (A') (A")
                (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=     1040327.
SCF Done:  E(RHF) =  -137.772939857     A.U. after    9 cycles
            Convg  =    0.7072D-08             -V/T =  2.0006
            S**2   =   0.0000
ExpMin= 1.15D-01 ExpMax= 9.99D+03 ExpMxC= 1.51D+03 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=         1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     3    32
Transform orbitals by the MOD method.
  Overlap analysis:     1 - Trace/N =  0.000540
                   Max |<i|i> - 1| =  0.004465
                   Max  <i|j>      =  0.003127
                   Min eigenvalue  =  0.995229
  Overlap analysis:     1 - Trace/N = -0.004495
                   Max |<i|i> - 1| =  0.043835
                   Max  <i|j>      =  0.015450
                   Min eigenvalue  =  0.935582
NBasis=    34 NAE=     8 NBE=     8 NFC=     2 NFV=     2
NROrb=     30 NOA=     6 NOB=     6 NVA=    24 NVB=    24
Non-canonical MOs are used.
No. of INTEGRALS =     57481 NBLK =        35 KOUNT =      1481
*****************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 2
```

```
*****************************************************************************
=================================================================
  STEP #PRES#  Generation of Linked Operators and Selection
=================================================================
== States to be calculated ==
           AG   AU
SINGLET    Yes  Yes
TRIPLET    No   No
IONIZED    No   No
ANIONIZED  No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  1)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
  ---------------------------------------------------------------
   During geometry optimization, the same linked and unlinked
   operators are used.
  ---------------------------------------------------------------
******************************
        SINGLET STATE
******************************
=================================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
=================================================================
=================================================================
  STEP #DIAGCI#  Solution of SDCI
=================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A'    CONVERGED
Solution for Singlet   A''   CONVERGED
=================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
=================================================================
=================================================================
  STEP #SAC#  Solution of SAC equation
=================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*******************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*******************************************
```

```
HF ENERGY     =    -137.772940 (AU)
SAC-NV  ENERGY=      -0.278972 (AU)
TOTAL ENERGY  =    -138.051912 (AU)
=====================================================================
  STEP #ULINTS#  Unlinked integral for Singlet Excited State (SAC-CI)
=====================================================================
==============================================================
  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
==============================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A''   CONVERGED
**********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
**********************************************
*******************************************************************************
Singlet       A''     ****************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    This state is being used for optimizations.
    Total energy       in au =    -137.984448
    Correlation energy in au =      -0.211509
    Excitation energy  in au =       0.067464    in eV =       1.835777
  *SINGLE EXCITATION
       8    9     0.95882         8   13    -0.20786
       7    9    -0.05952         4    9    -0.03690
  *DOUBLE EXCITATION
       8   23    8    9     0.06170         8   13    8   12    -0.05281
       8   14    8   13    -0.03806         6    9    5    9     0.03683
       8   23    4    9     0.03561         8    9    6    9     0.03304
       8   11    4    9     0.03062
==============================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
==============================================================
Energy gradient for SINGLET STATE A''  1-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-CI-V)=   -0.2115085367 Total energy=      -137.9844483936
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-CI-V / SAC-NV density.
Gamma from SAC-CI-V (singlet). Symmetry  2
Start back-transformation.
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     595
Number of TU pair in the last loop  =     595
```

SAC-CI result at the updated geometry. The total energy is decreasing compared with that at the last geometry (-137.984435 au).

```
Second-half back-transformation finished.
Solve CP equations for MOD among active MOs.
Max orbital gradient: YijMax=  0.001978 YabMax=  0.003142
DoAtom=TTT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      997720.
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
    1 vectors were produced by pass  8.
    1 vectors were produced by pass  9.
    1 vectors were produced by pass 10.
    1 vectors were produced by pass 11.
Inv2:  IOpt= 1 Iter= 1 AM= 4.44D-16 Conv= 1.00D-12.
Inverted reduced A of dimension   12 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6           0.000180782    0.000000000   -0.000355432
   2          9          -0.000004362    0.000000000    0.000539127
   3          1          -0.000176420    0.000000000   -0.000183695
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000539127 RMS     0.000239109

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Berny optimization.
Internal  Forces:  Max     0.000506399 RMS     0.000341784
Search for a local minimum.
Step number   3 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using D2CorX and points  1  2  3
Trust test= 8.71D-01 RLast= 1.38D-02 DXMaxT set to 3.00D-01
The second derivative matrix:
                         R1        R2        A1
          R1          0.64714
          R2         -0.01385   0.37779
          A1          0.03988   0.02876   0.18793
```

Energy gradient in cartesian coordinate calculated at the updated geometry.

```
    Eigenvalues ---    0.17998   0.38183   0.65105
RFO step:  Lambda=-3.55311650D-07.
Quartic linear search produced a step of -0.11462.
Iteration  1 RMS(Cart)=  0.00109961 RMS(Int)=  0.00000053
Iteration  2 RMS(Cart)=  0.00000043 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.47886   0.00051  -0.00006   0.00074   0.00069   2.47955
   R2        2.08463  -0.00001  -0.00019   0.00008  -0.00010   2.08453
   A1        2.15282   0.00031   0.00157  -0.00007   0.00150   2.15432
         Item               Value     Threshold  Converged?
Maximum Force            0.000506     0.000450     NO
RMS     Force            0.000342     0.000300     NO
Maximum Displacement     0.001116     0.001800     YES
RMS     Displacement     0.001099     0.001200     YES
Predicted change in Energy=-4.045137D-07
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
```

The largest remaining force is in the R1 (C-F distance).

Energy gradient does not satisfy convergence criteria.

```
                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6           0       -0.014324    0.000000    0.006630
   2          9           0       -0.003544    0.000000    1.318705
   3          1           0        0.901204    0.000000   -0.608677
---------------------------------------------------------------------
                   Distance matrix (angstroms):
                   1          2          3
    1  C    0.000000
    2  F    1.312119   0.000000
    3  H    1.103084   2.129171   0.000000
Stoichiometry    CHF
Framework group  CS[SG(CHF)]
Deg. of freedom     3
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6           0        0.057535    0.700081    0.000000
   2          9           0        0.057535   -0.612037    0.000000
   3          1           0       -0.863018    1.307846    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    710.4692271     34.3239051     32.7420827
Standard basis: D95(d) (6D, 7F)
```

The fourth geometry to be calculated.

```
There are    26 symmetry adapted basis functions of A'  symmetry.
There are     8 symmetry adapted basis functions of A"  symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   34 basis functions,    64 primitive gaussians,    34 cartesian basis functions
    8 alpha electrons        8 beta electrons
      nuclear repulsion energy        26.8933702917 Hartrees.
NAtoms=    3 NActive=    3 NUniq=    3 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    34 RedAO= T  NBF=    26     8
NBsUse=    34 1.00D-06 NBFU=    26     8
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A') (A') (A') (A') (A') (A") (A') (A')
      Virtual   (A") (A') (A') (A') (A") (A') (A') (A') (A") (A')
                (A') (A') (A") (A") (A') (A') (A') (A") (A') (A")
                (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=     1040327.
SCF Done:  E(RHF) =  -137.772767309     A.U. after    8 cycles
           Convg  =    0.6188D-08             -V/T =  2.0006
           S**2   =   0.0000
ExpMin= 1.15D-01 ExpMax= 9.99D+03 ExpMxC= 1.51D+03 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=         1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     3    32
Transform orbitals by the MOD method.
  Overlap analysis:     1 - Trace/N =  0.000561
                   Max |<i|i> - 1| =  0.004377
                   Max  <i|j>      =  0.003092
                   Min eigenvalue  =  0.995302
  Overlap analysis:     1 - Trace/N = -0.004558
                   Max |<i|i> - 1| =  0.043596
                   Max  <i|j>      =  0.016116
                   Min eigenvalue  =  0.935427
NBasis=    34 NAE=     8 NBE=     8 NFC=     2 NFV=     2
NROrb=     30 NOA=     6 NOB=     6 NVA=    24 NVB=    24
Non-canonical MOs are used.
No. of INTEGRALS =     57481 NBLK =        35 KOUNT =      1481
*******************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 3
*******************************************************************************
================================================================
  STEP #PRES#  Generation of Linked Operators and Selection
================================================================
```

```
== States to be calculated ==
           AG   AU
SINGLET    Yes  Yes
TRIPLET    No   No
IONIZED    No   No
ANIONIZED  No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  1)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
  ---------------------------------------------------------------
   During geometry optimization, the same linked and unlinked
   operators are used.
  ---------------------------------------------------------------
****************************
        SINGLET STATE
****************************
================================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A'    CONVERGED
Solution for Singlet   A''   CONVERGED
================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
================================================================
================================================================
  STEP #SAC#  Solution of SAC equation
================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*********************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*********************************************
HF ENERGY     =    -137.772767 (AU)
SAC-NV  ENERGY=      -0.278992 (AU)
TOTAL ENERGY  =    -138.051760 (AU)
====================================================================
```

```
  STEP #ULINTS#  Unlinked integral for Singlet Excited State (SAC-CI)
=====================================================================
=============================================================
  STEP #SCIV#  Iterative Diagonalization of SAC-CI-V
=============================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A''   CONVERGED
***********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
***********************************************
*****************************************************************************
Singlet       A''     ******************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    This state is being used for optimizations.
    Total energy       in au =    -137.984449
    Correlation energy in au =      -0.211682
    Excitation energy  in au =       0.067311    in eV =       1.831620
  *SINGLE EXCITATION
       8    9     0.95883         8   13    -0.20790
       7    9    -0.05908         4    9    -0.03711
  *DOUBLE EXCITATION
       8   23    8    9     0.06171         8   13    8   12    -0.05282
       8   14    8   13    -0.03805         6    9    5    9     0.03682
       8   23    4    9     0.03560         8    9    6    9     0.03304
       8   11    4    9     0.03058
=============================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
=============================================================
Energy gradient for SINGLET STATE A''  1-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-CI-V)=   -0.2116815098 Total energy=      -137.9844488183
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-CI-V / SAC-NV density.
Gamma from SAC-CI-V (singlet). Symmetry  2
Start back-transformation.
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     595
Number of TU pair in the last loop  =     595
Second-half back-transformation finished.
Solve CP equations for MOD among active MOs.
Max orbital gradient: YijMax=  0.001997 YabMax=  0.003147
DoAtom=TTT
```

SAC-CI result at the updated geometry. The total energy is decreasing compared with that at the last geometry (-137.984448 au).

```
        Differentiating once with respect to electric field.
              with respect to dipole field.
        Differentiating once with respect to nuclear coordinates.
        Store integrals in memory, NReq=      997720.
        There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
    1 vectors were produced by pass  8.
    1 vectors were produced by pass  9.
    1 vectors were produced by pass 10.
    1 vectors were produced by pass 11.
Inv2:  IOpt= 1 Iter= 1 AM= 6.78D-16 Conv= 1.00D-12.
Inverted reduced A of dimension   12 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6          -0.000022230    0.000000000   -0.000034218
   2          9           0.000138837    0.000000000    0.000107313
   3          1          -0.000116607    0.000000000   -0.000073096
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000138837 RMS     0.000075570

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.000069065 RMS     0.000040227
Search for a local minimum.
Step number   4 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using D2CorX and points  1  2  3  4
Trust test= 1.05D+00 RLast= 1.65D-03 DXMaxT set to 3.00D-01
The second derivative matrix:
                          R1        R2        A1
          R1           0.57585
          R2          -0.00511   0.37764
          A1           0.02710   0.03080   0.19382
    Eigenvalues ---    0.18684   0.38266   0.57781
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of  0.06786.
Iteration  1 RMS(Cart)=  0.00005159 RMS(Int)=  0.00000000
```

Energy gradient in cartesian coordinate calculated at the updated geometry.

```
Iteration  2 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.47955   0.00007   0.00005   0.00007   0.00012   2.47967
   R2        2.08453  -0.00001  -0.00001  -0.00002  -0.00002   2.08450
   A1        2.15432   0.00000   0.00010  -0.00011   0.00000   2.15432
        Item               Value     Threshold  Converged?
Maximum Force            0.000069     0.000450     YES
RMS     Force            0.000040     0.000300     YES
Maximum Displacement     0.000070     0.001800     YES
RMS     Displacement     0.000052     0.001200     YES
Predicted change in Energy=-4.243675D-09
Optimization completed.
   -- Stationary point found.
                          ----------------------------
                          !   Optimized Parameters   !
                          ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.3121         -DE/DX =    0.0001              !
! R2    R(1,3)                  1.1031         -DE/DX =    0.0                 !
! A1    A(2,1,3)              123.4335         -DE/DX =    0.0                 !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6          0        -0.014324    0.000000    0.006630
   2          9          0        -0.003544    0.000000    1.318705
   3          1          0         0.901204    0.000000   -0.608677
---------------------------------------------------------------------
                   Distance matrix (angstroms):
                   1          2          3
    1  C    0.000000
    2  F    1.312119   0.000000
    3  H    1.103084   2.129171   0.000000
Stoichiometry    CHF
Framework group  CS[SG(CHF)]
Deg. of freedom     3
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
```

Convergence achieved.

Optimized parameters

```
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6           0        0.057535    0.700081    0.000000
   2          9           0        0.057535   -0.612037    0.000000
   3          1           0       -0.863018    1.307846    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):     710.4692271     34.3239051     32.7420827

*********************************************************************

           Population analysis using the SCF density.

*********************************************************************

Orbital symmetries:
      Occupied  (A') (A') (A') (A') (A') (A″) (A') (A')
      Virtual   (A″) (A') (A') (A') (A″) (A') (A') (A') (A″) (A')
                (A') (A') (A″) (A″) (A') (A') (A') (A″) (A') (A″)
                (A') (A') (A') (A') (A') (A')
The electronic state is 1-A'.
Alpha  occ. eigenvalues --  -26.35882 -11.36667  -1.67686  -0.92120  -0.76388
Alpha  occ. eigenvalues --   -0.71414  -0.69858  -0.37567
Alpha virt. eigenvalues --    0.07060   0.24847   0.35205   0.42819   0.49311
Alpha virt. eigenvalues --    0.59729   0.67590   1.00995   1.11243   1.16343
Alpha virt. eigenvalues --    1.21701   1.41615   1.73859   1.77990   1.78723
Alpha virt. eigenvalues --    2.08493   2.27300   2.36110   2.40139   2.84229
Alpha virt. eigenvalues --    2.93173   3.20454   4.03237   4.37104  27.38067
Alpha virt. eigenvalues --   56.51010
         Condensed to atoms (all electrons):
             1          2          3
    1  C    5.505419   0.217239   0.239995
    2  F    0.217239   8.998677  -0.020684
    3  H    0.239995  -0.020684   0.622804
Mulliken atomic charges:
             1
    1  C    0.037347
    2  F   -0.195232
    3  H    0.157885
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  C    0.195232
    2  F   -0.195232
    3  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    56.8363
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=    -1.9196    Y=     0.4170    Z=     0.0000  Tot=     1.9644
```

```
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=   -12.2644   YY=   -11.8035   ZZ=   -10.0294
  XY=    -2.3852   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -0.8987   YY=    -0.4377   ZZ=     1.3364
  XY=    -2.3852   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=    -1.9805  YYY=    -6.8990  ZZZ=     0.0000  XYY=    -3.2616
 XXY=    -3.1707  XXZ=     0.0000  XZZ=    -0.5313  YZZ=    -1.5720
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=   -15.9074 YYYY=   -44.5006 ZZZZ=    -7.4762 XXXY=    -0.3318
XXXZ=     0.0000 YYYX=    -2.9252 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=   -10.8281 XXZZ=    -3.9552 YYZZ=    -8.5511
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0955
N-N= 2.689337029169D+01 E-N=-3.812640098822D+02  KE= 1.376833820922D+02
Symmetry A'   KE= 1.317704191491D+02
Symmetry A"   KE= 5.912962943143D+00
Final structure in terms of initial Z-matrix:
C
F,1,FC
H,1,HC,2,HCF
     Variables:
FC=1.31211872
HC=1.1030842
HCF=123.43347556

Test job not archived.
1¥1¥GINC-MIRAI86¥FOpt¥RSACCI¥D95(d)¥C1H1F1¥MASAHIRO¥03-Aug-2004¥0¥¥# S
AC-CI(SINGLET=(NSTATE=(0,1)), TARGETSTATE=(SPINSTATE=SINGLET,SYMMETRY=
2,ROOT=1)) /D95(D) OPT TEST¥¥Gaussian Test Job 638 (Part 1): SAC-CI SD
-R geometry optimization for the singlet ground (A') and A" excited st
ate of HCF with D95(d) basis. Minimum-Orbital Deformation (MOD) method
 is used and full-valence active MOs are adopted (FC; default). First
is the geometry optimization for the excited A" state. Initial geometr
y is the experimental one. The results are compared with experiments i
n Part I-L of the SAC-CI Guide.¥¥0,1¥C,-0.0632841718,0.,-0.6995851892¥
F,-0.0525043491,0.,0.6124892491¥H,0.8522441722,0.,-1.3148921068¥¥Versi
on=AI64T-G03RevC.02¥State=1-A'¥HF=-137.7727673¥RMSD=6.188e-09¥RMSF=7.5
57e-05¥Dipole=0.474704,0.,-0.2678052¥PG=CS [SG(C1H1F1)]¥¥@


You never know when you're making a memory.
                        -- Rickie Lee Jones
Job cpu time:  0 days  0 hours  8 minutes 34.9 seconds.
File lengths (MBytes):  RWF=    590 Int=      0 D2E=      0 Chk=     10 Scr=     19
Normal termination of Gaussian 03 at Tue Aug  3 13:25:58 2004.
Initial command:
/work/g03.C02/g03/l1.exe /work/g03.C02/inputs/Gau-184914.inp -scrdir=/work/g03.C02/inputs/
```

```
Entering Link 1 = /work/g03.C02/g03/l1.exe PID=    184996.

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```
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K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,
A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

******************************************
Gaussian 03:  AI64T-G03RevC.02 12-Jun-2004
                 3-Aug-2004
******************************************
%mem=12mw
---------------------------------------------------------------------
# SAC-CI(SacOnly, TargetState=(SpinState=Singlet,Symmetry=1,Root=0)) /
D95(d) Opt test
---------------------------------------------------------------------
1/18=20,38=1/1,3;
2/9=110,17=6,18=5,40=1/2;
3/5=8,7=1,11=9,16=1,25=1,30=1,36=2/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=5,9=30000,10=1,40=1,41=2,42=2/1,4;
9/15=1/23;
11/28=-13,29=200,42=3,46=2/11;
10/5=5/2;
6/7=2,8=2,9=2,10=2/1;
7/12=7/1,2,3,16;
1/18=20/3(1);
99//99;
2/9=110/2;
3/5=8,7=1,11=9,16=1,25=1,30=1,36=2/1,2,3;
4/5=5,16=3/1;
5/5=2,38=5/2;
```

This time, structure of the ground state is optimized with the SAC method. “SACOnly” requests only ground-state calculation, and “Root=0” means that the target state is the ground state.

```
8/6=5,9=30000,10=1,40=1,41=2,42=2/1,4;
9/15=1/23;
11/28=-13,29=200,42=3,46=2/11;
10/5=5/2;
7/12=7/1,2,3,16;
1/18=20/3(-9);
2/9=110/2;
6/7=2,8=2,9=2,10=2/1;
99//99;
-----------------------------------------------------------------------
Gaussian Test Job 638 (Part 2): Geometry optimization of the SAC groun
d state of HCF. Initial geometry is the experimental one. MacroIter=1
(default).
-----------------------------------------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C
F                    1    FC
H                    1    HC       2    HCF
      Variables:
 FC                    1.305
 HC                    1.138
 HCF                 104.1
```

Nuclear coordinates for HCF given in the Gaussian input

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                          ----------------------------
                          !    Initial Parameters    !
                          ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
-------------------------------------------------------------------------------
! R1    R(1,2)                   1.305          estimate D2E/DX2                !
! R2    R(1,3)                   1.138          estimate D2E/DX2                !
! A1    A(2,1,3)               104.1            estimate D2E/DX2                !
-------------------------------------------------------------------------------
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6          0        0.000000    0.000000    0.000000
   2          9          0        0.000000    0.000000    1.305000
```

Definition of the variables and initial values.

```
   3          1             0        1.103714    0.000000   -0.277234
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3
    1  C    0.000000
    2  F    1.305000   0.000000
    3  H    1.138000   1.929158   0.000000
Stoichiometry    CHF
Framework group  CS[SG(CHF)]
Deg. of freedom     3
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0        0.068982    0.716735    0.000000
   2          9             0        0.068982   -0.588265    0.000000
   3          1             0       -1.034732    0.993969    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    467.0805987     36.7163219     34.0404653
Standard basis: D95(d) (6D, 7F)
There are    26 symmetry adapted basis functions of A'  symmetry.
There are     8 symmetry adapted basis functions of A"  symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   34 basis functions,    64 primitive gaussians,    34 cartesian basis functions
    8 alpha electrons        8 beta electrons
      nuclear repulsion energy        27.1557690924 Hartrees.
NAtoms=    3 NActive=    3 NUniq=    3 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    34 RedAO= T  NBF=    26     8
NBsUse=    34 1.00D-06 NBFU=    26     8
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.15D-01 ExpMax= 9.99D+03 ExpMxC= 1.51D+03 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=         1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Initial guess orbital symmetries:
      Occupied  (A') (A') (A') (A') (A') (A") (A') (A')
      Virtual   (A") (A') (A') (A') (A") (A') (A') (A') (A") (A')
                (A') (A') (A") (A') (A") (A') (A') (A") (A') (A')
                (A") (A') (A') (A') (A') (A')
The electronic state of the initial guess is 1-A'.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
```

```
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=     1040327.
SCF Done:  E(RHF) =  -137.791946524     A.U. after   12 cycles
            Convg  =    0.2255D-08             -V/T =  2.0006
            S**2   =   0.0000
ExpMin= 1.15D-01 ExpMax= 9.99D+03 ExpMxC= 1.51D+03 IAcc=1 IRadAn=        1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=        1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     3    32
Use canonical orbitals as reference of MOD.
  Overlap analysis:     1 - Trace/N =  0.000000
                    Max |<i|i> - 1| =  0.000000
                    Max  <i|j>      =  0.000000
                    Min eigenvalue  =  1.000000
  Overlap analysis:     1 - Trace/N =  0.000000
                    Max |<i|i> - 1| =  0.000000
                    Max  <i|j>      =  0.000000
                    Min eigenvalue  =  1.000000
NBasis=    34 NAE=     8 NBE=     8 NFC=     2 NFV=     2
NROrb=     30 NOA=     6 NOB=     6 NVA=    24 NVB=    24
-----------------------------------------------------------------------
#######################################################################
-----------------------------------------------------------------------
              SAC/SAC-CI Program Combined with GAUSSIAN
                            for Calculating
        Ground, Excited, Ionized, and Electron-Attached States
                                and
            Singlet, Doublet, Triplet, Quartet, Quintet,
                  Sextet, and Septet Spin States
                                and
                 Their Analytical Energy Gradients
                       coded originally by
                        Hiroshi Nakatsuji
                         and extended by
 H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa,
      M. Ishida, T. Nakajima, Y. Honda, O. Kitao, and H. Nakai
                                at
                 Department of Hydrocarbon Chemistry,
               Division of Molecular Engineering, and
      Department of Synthetic Chemistry & Biological Chemistry,
                  Graduate School of Engineering,
                        Kyoto University,
                      Kyoto 606-8501, Japan
-----------------------------------------------------------------------
#######################################################################
-----------------------------------------------------------------------
No. of INTEGRALS =     57481 NBLK =        35 KOUNT =      1481
*****************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 0
```

```
*****************************************************************************
==================================================================
  STEP #PRES#  Generation of Linked Operators and Selection
==================================================================
== States to be calculated ==
           AG   AU
SINGLET    Yes  No
TRIPLET    No   No
IONIZED    No   No
ANIONIZED  No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  0)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
****************************
        SINGLET STATE
****************************
------------------------------------------------------------
LINKED OPERATORS FOR SAC:    SYMMETRY = A'  GROUND STATE
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            92        5656         5748
    AFTER             92        4164         4257
==================================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
==================================================================
==================================================================
  STEP #DIAGCI#  Solution of SDCI
==================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A'    CONVERGED
==================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
==================================================================
Threshold for S2 operator (CThreULS2G) 0.500D-02
==================================================================
  STEP #SAC#  Solution of SAC equation
==================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*********************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
```

Perturbation selection only for the ground state. Number of the linked operators for single- and double-excitation operators in SAC w.f. before and after the perturbation selection

Result of SAC calculation. Hartree-Fock (HF) energy, SAC-NV energy (correlation energy obtained with the SAC method), and the SAC-NV coefficients are shown. HF configuration always has 1.00 in the SAC wave function.

```
*****************************************
HF ENERGY     =    -137.791947 (AU)
SAC-NV  ENERGY=      -0.280138 (AU)
TOTAL ENERGY  =    -138.072084 (AU)
SAC-NV  coefficients (|C|>=0.03)
*SINGLE EXCITATION
       6    9      0.05549
*DOUBLE EXCITATION
       8    9    8    9     -0.08094         8    9    7    9      0.05818
       8   13    8    9      0.05663         6   17    6    9     -0.05554
       8    9    4    9     -0.04847         6   17    5   18     -0.04549
       8   23    8    9     -0.04415         8   14    8   12     -0.03943
       6   17    6   17     -0.03861         7    9    4    9      0.03844
       6    9    6    9     -0.03816         8   14    7   14      0.03385
       6   17    4   16     -0.03375         8   15    8   10     -0.03142
       7   14    6    9     -0.03108         8   11    8   11     -0.03095
       6    9    4   15      0.03088         8   11    7   11     -0.03082
       8   11    8   10      0.03053
Hartree-Fock configuration   1.00000
================================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
================================================================
Energy gradient for SINGLET STATE A'   0-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-NV)=   -0.2801376643 Total energy=      -138.0720841882
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-NV density.
Start back-transformation.
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     595
Number of TU pair in the last loop  =     595
Second-half back-transformation finished.
Solve CP equations for MOD among active MOs.
Max orbital gradient: YijMax=  0.000946 YabMax=  0.000671
DoAtom=TTT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      997720.
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
```

Solving Z-vector equation for the target state.

```
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
    1 vectors were produced by pass  8.
    1 vectors were produced by pass  9.
    1 vectors were produced by pass 10.
Inv2:  IOpt= 1 Iter= 1 AM= 3.90D-16 Conv= 1.00D-12.
Inverted reduced A of dimension   11 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.

**********************************************************************

           Population analysis using the SCF density.

**********************************************************************

Orbital symmetries:
      Occupied  (A') (A') (A') (A') (A') (A″) (A') (A')
      Virtual   (A″) (A') (A') (A') (A″) (A') (A') (A') (A″) (A')
                (A') (A') (A″) (A') (A″) (A') (A') (A″) (A') (A″)
                (A') (A') (A') (A') (A') (A')
The electronic state is 1-A'.
Alpha  occ. eigenvalues --  -26.35513 -11.37461  -1.68192  -0.92620  -0.76430
Alpha  occ. eigenvalues --   -0.71460  -0.66784  -0.40444
Alpha virt. eigenvalues --    0.07105   0.25841   0.32638   0.42576   0.49083
Alpha virt. eigenvalues --    0.63675   0.66904   1.00911   1.11343   1.12589
Alpha virt. eigenvalues --    1.19547   1.41828   1.74751   1.76759   1.77038
Alpha virt. eigenvalues --    2.04953   2.32267   2.36043   2.47213   2.85235
Alpha virt. eigenvalues --    2.85588   3.21163   4.01717   4.38529  27.37302
Alpha virt. eigenvalues --   56.51935
         Condensed to atoms (all electrons):
             1          2          3
    1  C    5.412807   0.228755   0.277592
    2  F    0.228755   9.013329  -0.044807
    3  H    0.277592  -0.044807   0.650784
Mulliken atomic charges:
             1
    1  C    0.080846
    2  F   -0.197277
    3  H    0.116431
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  C    0.197277
    2  F   -0.197277
    3  H    0.000000
```

```
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    55.3866
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=    -1.5659    Y=     0.1393    Z=     0.0000  Tot=     1.5720
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=   -11.7869   YY=   -12.6590   ZZ=   -10.0557
  XY=    -1.8680   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -0.2864   YY=    -1.1584   ZZ=     1.4448
  XY=    -1.8680   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=    -1.6245  YYY=    -8.6208  ZZZ=     0.0000  XYY=    -2.4665
 XXY=    -2.9407  XXZ=     0.0000  XZZ=    -0.3227  YZZ=    -1.6028
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=   -16.2695 YYYY=   -44.9942 ZZZZ=    -7.4748 XXXY=    -0.2102
XXXZ=     0.0000 YYYX=    -1.6945 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=   -10.6832 XXZZ=    -4.0943 YYZZ=    -8.1525
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.1734
N-N= 2.715576909245D+01 E-N=-3.818326179444D+02  KE= 1.377152681615D+02
Symmetry A'   KE= 1.318427655260D+02
Symmetry A"   KE= 5.872502635478D+00
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6           0.000968947    0.000000000   -0.018989500
   2          9           0.003034084    0.000000000    0.012788334
   3          1          -0.004003030    0.000000000    0.006201166
-------------------------------------------------------------------
Cartesian Forces:  Max     0.018989500 RMS     0.008088166

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.013079888 RMS     0.009858270
Search for a local minimum.
Step number   1 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- first step.
The second derivative matrix:
                          R1        R2        A1
          R1           0.65823
          R2           0.00000   0.29807
          A1           0.00000   0.00000   0.16000
    Eigenvalues ---    0.16000   0.29807   0.65823
RFO step:  Lambda=-9.14091009D-04.
Linear search not attempted -- first point.
```

Energy gradient in cartesian coordinate calculated at the initial geometry.

```
Iteration  1 RMS(Cart)=  0.04255573 RMS(Int)=  0.00089377
Iteration  2 RMS(Cart)=  0.00069602 RMS(Int)=  0.00000002
Iteration  3 RMS(Cart)=  0.00000002 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1         2.46609   0.01308   0.00000   0.01984   0.01984   2.48594
   R2         2.15051  -0.00573   0.00000  -0.01916  -0.01916   2.13135
   A1         1.81689  -0.00936   0.00000  -0.05819  -0.05819   1.75870
        Item               Value     Threshold  Converged?
Maximum Force            0.013080     0.000450     NO
RMS     Force            0.009858     0.000300     NO
Maximum Displacement     0.047337     0.001800     NO
RMS     Displacement     0.042830     0.001200     NO
Predicted change in Energy=-4.589406D-04
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6           0       -0.009298    0.000000   -0.017622
   2          9           0        0.019109    0.000000    1.297572
   3          1           0        1.093904    0.000000   -0.252184
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3
    1  C    0.000000
    2  F    1.315501   0.000000
    3  H    1.127863   1.885982   0.000000
Stoichiometry    CHF
Framework group  CS[SG(CHF)]
Deg. of freedom     3
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6           0        0.069251    0.726801    0.000000
   2          9           0        0.069251   -0.588699    0.000000
   3          1           0       -1.038759    0.937486    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    458.3559827     36.5353205     33.8381026
Standard basis: D95(d) (6D, 7F)
There are    26 symmetry adapted basis functions of A'  symmetry.
There are     8 symmetry adapted basis functions of A"  symmetry.
```

The largest remaining force is in the R1 (C-F distance).

Energy gradient and displacements do not satisfy convergence criteria.

The second geometry to be calculated.

```
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   34 basis functions,    64 primitive gaussians,    34 cartesian basis functions
    8 alpha electrons        8 beta electrons
      nuclear repulsion energy        27.0625732077 Hartrees.
NAtoms=    3 NActive=    3 NUniq=    3 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    34 RedAO= T  NBF=    26     8
NBsUse=    34 1.00D-06 NBFU=    26     8
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A') (A') (A') (A') (A') (A") (A') (A')
      Virtual   (A") (A') (A') (A') (A") (A') (A') (A') (A") (A')
                (A') (A') (A") (A') (A") (A') (A') (A") (A') (A")
                (A') (A') (A') (A') (A') (A')
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.15D-01 ExpMax= 9.99D+03 ExpMxC= 1.51D+03 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=         1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=     1040327.
SCF Done:  E(RHF) =  -137.791992617     A.U. after   10 cycles
            Convg  =    0.5502D-08             -V/T =  2.0005
            S**2   =   0.0000
ExpMin= 1.15D-01 ExpMax= 9.99D+03 ExpMxC= 1.51D+03 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=         1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     3    32
Transform orbitals by the MOD method.
  Overlap analysis:     1 - Trace/N = -0.000070
                    Max |<i|i> - 1| =  0.004049
                    Max  <i|j>      =  0.005785
                    Min eigenvalue  =  0.991440
  Overlap analysis:     1 - Trace/N = -0.001021
                    Max |<i|i> - 1| =  0.020584
                    Max  <i|j>      =  0.023455
                    Min eigenvalue  =  0.959351
NBasis=    34 NAE=     8 NBE=     8 NFC=     2 NFV=     2
NROrb=     30 NOA=     6 NOB=     6 NVA=    24 NVB=    24
Non-canonical MOs are used.
No. of INTEGRALS =     57481 NBLK =        35 KOUNT =      1481
*******************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 1
*******************************************************************************
==============================================================
```

MOD transformation within occupied and virtural block MOs. Checking the "displaced" overlap matrix elements. See section I-D-8 for details.

```
  STEP #PRES#  Generation of Linked Operators and Selection
================================================================
== States to be calculated ==
           AG   AU
SINGLET    Yes  No
TRIPLET    No   No
IONIZED    No   No
ANIONIZED  No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  0)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
  ---------------------------------------------------------------
   During geometry optimization, the same linked and unlinked
   operators are used.
  ---------------------------------------------------------------
******************************
        SINGLET STATE
******************************
================================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A'    CONVERGED
================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
================================================================
================================================================
  STEP #SAC#  Solution of SAC equation
================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*********************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*********************************************
HF ENERGY     =    -137.791993 (AU)
SAC-NV  ENERGY=      -0.280355 (AU)
TOTAL ENERGY  =    -138.072347 (AU)
```

SAC result at the updated geometry. The total energy is decreasing compared with that at the last geometry (-138.072084 au)

```
SAC-NV  coefficients (|C|>=0.03)
*SINGLE EXCITATION
       6    9      0.05644
*DOUBLE EXCITATION
       8    9    8    9     -0.07966         8    9    7    9      0.05795
       8   13    8    9      0.05618         6   17    6    9     -0.05563
       8    9    4    9     -0.04921         6   17    5   18     -0.04567
       8   23    8    9     -0.04410         7    9    4    9      0.03908
       8   14    8   12     -0.03882         6   17    6   17     -0.03874
       6    9    6    9     -0.03820         8   14    7   14      0.03414
       6   17    4   16     -0.03382         8   15    8   10     -0.03211
       6    9    4   15      0.03091         7   14    6    9     -0.03075
       8   11    8   10      0.03056         8   11    8   11     -0.03036
Hartree-Fock configuration   1.00000
================================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
================================================================
Energy gradient for SINGLET STATE A'   0-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-NV)=   -0.2803546750 Total energy=      -138.0723472918
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-NV density.
Start back-transformation.
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     595
Number of TU pair in the last loop  =     595
Second-half back-transformation finished.
Solve CP equations for MOD among active MOs.
Max orbital gradient: YijMax=  0.000928 YabMax=  0.000668
DoAtom=TTT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      997720.
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
```

```
    1 vectors were produced by pass  7.
    1 vectors were produced by pass  8.
    1 vectors were produced by pass  9.
    1 vectors were produced by pass 10.
Inv2:  IOpt= 1 Iter= 1 AM= 3.09D-16 Conv= 1.00D-12.
Inverted reduced A of dimension   11 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6           0.005713090    0.000000000   -0.004155712
   2          9          -0.005103896    0.000000000    0.007353799
   3          1          -0.000609194    0.000000000   -0.003198087
-------------------------------------------------------------------
Cartesian Forces:  Max     0.007353799 RMS     0.003953006

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.009579182 RMS     0.007136421
Search for a local minimum.
Step number   2 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using D2CorX and points  1  2
Trust test= 5.73D-01 RLast= 6.44D-02 DXMaxT set to 3.00D-01
The second derivative matrix:
                          R1        R2        A1
          R1           0.49223
          R2           0.06105   0.28261
          A1           0.05687   0.01639   0.33954
    Eigenvalues ---    0.26611   0.32091   0.52736
RFO step:  Lambda=-2.43490838D-04.
Quartic linear search produced a step of -0.29814.
Iteration  1 RMS(Cart)=  0.02126230 RMS(Int)=  0.00016135
Iteration  2 RMS(Cart)=  0.00012005 RMS(Int)=  0.00000000
Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1         2.48594   0.00779  -0.00592   0.01955   0.01363   2.49957
   R2         2.13135  -0.00057   0.00571  -0.01222  -0.00651   2.12484
   A1         1.75870   0.00958   0.01735   0.00879   0.02613   1.78483
        Item               Value     Threshold  Converged?
Maximum Force            0.009579     0.000450     NO
RMS     Force            0.007136     0.000300     NO
Maximum Displacement     0.021867     0.001800     NO
RMS     Displacement     0.021226     0.001200     NO
Predicted change in Energy=-1.805374D-04
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
```

Energy gradient in cartesian coordinate calculated at the updated geometry.

The largest remaining force is in the A1 (H-C-F angle).

Energy gradient and displacements do not satisfy convergence criteria.

The next geometry to be calculated.

```
                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6            0       -0.001412    0.000000   -0.015572
   2          9            0        0.009853    0.000000    1.307094
   3          1            0        1.095273    0.000000   -0.263756
---------------------------------------------------------------------
                   Distance matrix (angstroms):
                   1          2          3
    1  C    0.000000
    2  F    1.322714   0.000000
    3  H    1.124417   1.909373   0.000000
Stoichiometry    CHF
Framework group  CS[SG(CHF)]
Deg. of freedom     3
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6            0        0.068672    0.729099    0.000000
   2          9            0        0.068672   -0.593614    0.000000
   3          1            0       -1.030087    0.967934    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    467.9832111     35.9930492     33.4224925
Standard basis: D95(d) (6D, 7F)
There are    26 symmetry adapted basis functions of A'  symmetry.
There are     8 symmetry adapted basis functions of A"  symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   34 basis functions,    64 primitive gaussians,    34 cartesian basis functions
    8 alpha electrons        8 beta electrons
      nuclear repulsion energy        26.9218120889 Hartrees.
NAtoms=    3 NActive=    3 NUniq=    3 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    34 RedAO= T  NBF=    26     8
NBsUse=    34 1.00D-06 NBFU=    26     8
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A') (A') (A') (A') (A') (A") (A') (A')
      Virtual   (A") (A') (A') (A') (A") (A') (A') (A') (A") (A')
                (A') (A') (A") (A') (A") (A') (A') (A") (A') (A")
```

```
                (A') (A') (A') (A') (A') (A')
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.15D-01 ExpMax= 9.99D+03 ExpMxC= 1.51D+03 IAcc=1 IRadAn=        1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=        1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=     1040327.
SCF Done:  E(RHF) =  -137.791962143     A.U. after    9 cycles
           Convg  =    0.9381D-08             -V/T =  2.0007
           S**2   =   0.0000
ExpMin= 1.15D-01 ExpMax= 9.99D+03 ExpMxC= 1.51D+03 IAcc=1 IRadAn=        1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=        1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     3    32
Transform orbitals by the MOD method.
  Overlap analysis:     1 - Trace/N = -0.000034
                   Max |<i|i> - 1| =  0.003450
                   Max  <i|j>      =  0.003447
                   Min eigenvalue  =  0.994572
  Overlap analysis:     1 - Trace/N = -0.002007
                   Max |<i|i> - 1| =  0.020138
                   Max  <i|j>      =  0.015449
                   Min eigenvalue  =  0.961930
NBasis=    34 NAE=     8 NBE=     8 NFC=     2 NFV=     2
NROrb=     30 NOA=     6 NOB=     6 NVA=    24 NVB=    24
Non-canonical MOs are used.
No. of INTEGRALS =     57481 NBLK =        35 KOUNT =      1481
*******************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 2
*******************************************************************************
================================================================
  STEP #PRES#  Generation of Linked Operators and Selection
================================================================
== States to be calculated ==
           AG   AU
SINGLET    Yes  No
TRIPLET    No   No
IONIZED    No   No
ANIONIZED  No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  0)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
  ------------------------------------------------------------
```

```
   During geometry optimization, the same linked and unlinked
   operators are used.
  ------------------------------------------------------------
****************************
        SINGLET STATE
****************************
==============================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
==============================================================
==============================================================
  STEP #DIAGCI#  Solution of SDCI
==============================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A'    CONVERGED
==============================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
==============================================================
==============================================================
  STEP #SAC#  Solution of SAC equation
==============================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*********************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*********************************************
HF ENERGY     =    -137.791962 (AU)
SAC-NV  ENERGY=      -0.280541 (AU)
TOTAL ENERGY  =    -138.072503 (AU)
SAC-NV  coefficients (|C|>=0.03)
*SINGLE EXCITATION
       6    9      0.05697
*DOUBLE EXCITATION
       8    9    8    9     -0.08067         8    9    7    9      0.05860
       8   13    8    9      0.05679         6   17    6    9     -0.05548
       8    9    4    9     -0.04885         6   17    5   18     -0.04580
       8   23    8    9     -0.04412         7    9    4    9      0.03894
       8   14    8   12     -0.03893         6   17    6   17     -0.03883
       6    9    6    9     -0.03791         8   14    7   14      0.03423
       6   17    4   16     -0.03388         8   15    8   10     -0.03220
       7   14    6    9     -0.03118         6    9    4   15      0.03098
       8   11    8   10      0.03006
Hartree-Fock configuration   1.00000
==============================================================
```

By combined use of GSUM and MOD method equivalent sets of linked and unlinked terms are used during optimization. No new perturbation selection carried out.

SAC result at the updated geometry. The total energy is decreasing compared with that at the last geometry (-138.072347 au)

```
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
=================================================================
Energy gradient for SINGLET STATE A'   0-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-NV)=   -0.2805412025 Total energy=      -138.0725033455
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-NV density.
Start back-transformation.
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     595
Number of TU pair in the last loop  =     595
Second-half back-transformation finished.
Solve CP equations for MOD among active MOs.
Max orbital gradient: YijMax=  0.000941 YabMax=  0.000694
DoAtom=TTT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      997720.
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
    1 vectors were produced by pass  8.
    1 vectors were produced by pass  9.
    1 vectors were produced by pass 10.
Inv2:  IOpt= 1 Iter= 1 AM= 3.58D-16 Conv= 1.00D-12.
Inverted reduced A of dimension   11 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6          -0.001078012    0.000000000    0.000597404
   2          9          -0.000681617    0.000000000   -0.001531577
   3          1           0.001759629    0.000000000    0.000934172
```

Energy gradient in cartesian coordinate calculated at the updated geometry.

```
---------------------------------------------------------------------------
Cartesian Forces:  Max     0.001759629 RMS     0.000960226

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Berny optimization.
Internal  Forces:  Max     0.001150344 RMS     0.001031092
Search for a local minimum.
Step number   3 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using D2CorX and points  1  2  3
Trust test= 8.64D-01 RLast= 3.02D-02 DXMaxT set to 3.00D-01
The second derivative matrix:
                          R1        R2        A1
          R1           0.51481
          R2           0.02637   0.29965
          A1           0.08020  -0.00131   0.35759
    Eigenvalues ---    0.29319   0.32811   0.55076
RFO step:  Lambda=-2.98242902D-06.
Quartic linear search produced a step of -0.11372.
Iteration  1 RMS(Cart)=  0.00208820 RMS(Int)=  0.00000149
Iteration  2 RMS(Cart)=  0.00000113 RMS(Int)=  0.00000000
Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X      New X
                                (Linear)    (Quad)   (Total)
   R1         2.49957  -0.00115  -0.00155  -0.00059  -0.00214   2.49743
   R2         2.12484   0.00105   0.00074   0.00298   0.00372   2.12856
   A1         1.78483  -0.00087  -0.00297   0.00097  -0.00200   1.78283
        Item               Value     Threshold  Converged?
Maximum Force            0.001150     0.000450     NO
RMS     Force            0.001031     0.000300     NO
Maximum Displacement     0.002481     0.001800     NO
RMS     Displacement     0.002089     0.001200     NO
Predicted change in Energy=-4.011233D-06
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                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6           0       -0.002725    0.000000   -0.015256
   2          9           0        0.010415    0.000000    1.306261
   3          1           0        1.096024    0.000000   -0.263239
---------------------------------------------------------------------
                    Distance matrix (angstroms):
                    1          2          3
    1  C    0.000000
    2  F    1.321582   0.000000
    3  H    1.126386   1.908370   0.000000
```

The largest remaining force is in the R1 (C-F distance).

Energy gradient and displacements do not satisfy convergence criteria.

The next geometry to be calculated.

```
Stoichiometry    CHF
Framework group  CS[SG(CHF)]
Deg. of freedom     3
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6            0        0.068823    0.728575    0.000000
   2          9            0        0.068823   -0.593008    0.000000
   3          1            0       -1.032338    0.965621    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    465.8491572     36.0620779     33.4710352
Standard basis: D95(d) (6D, 7F)
There are    26 symmetry adapted basis functions of A'  symmetry.
There are     8 symmetry adapted basis functions of A"  symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   34 basis functions,    64 primitive gaussians,    34 cartesian basis functions
    8 alpha electrons        8 beta electrons
      nuclear repulsion energy        26.9366849068 Hartrees.
NAtoms=    3 NActive=    3 NUniq=    3 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    34 RedAO= T  NBF=    26     8
NBsUse=    34 1.00D-06 NBFU=    26     8
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (A') (A') (A') (A') (A') (A") (A') (A')
      Virtual   (A") (A') (A') (A') (A") (A') (A') (A') (A") (A')
                (A') (A') (A") (A') (A") (A') (A') (A") (A') (A")
                (A') (A') (A') (A') (A') (A')
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=     1040327.
SCF Done:  E(RHF) =  -137.791956388     A.U. after    8 cycles
            Convg  =    0.9002D-08             -V/T =  2.0007
            S**2   =   0.0000
ExpMin= 1.15D-01 ExpMax= 9.99D+03 ExpMxC= 1.51D+03 IAcc=1 IRadAn=         1 AccDes= 1.00D-06
HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=         1 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     3    32
Transform orbitals by the MOD method.
  Overlap analysis:     1 - Trace/N = -0.000017
```

```
                    Max |<i|i> - 1| =  0.003524
                    Max  <i|j>      =  0.003594
                    Min eigenvalue  =  0.994434
  Overlap analysis:     1 - Trace/N = -0.001987
                    Max |<i|i> - 1| =  0.018178
                    Max  <i|j>      =  0.014745
                    Min eigenvalue  =  0.963062
NBasis=    34 NAE=     8 NBE=     8 NFC=     2 NFV=     2
NROrb=     30 NOA=     6 NOB=     6 NVA=    24 NVB=    24
Non-canonical MOs are used.
No. of INTEGRALS =     57481 NBLK =        35 KOUNT =      1481
*******************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 3
*******************************************************************************
================================================================
  STEP #PRES#  Generation of Linked Operators and Selection
================================================================
== States to be calculated ==
           AG   AU
SINGLET    Yes  No
TRIPLET    No   No
IONIZED    No   No
ANIONIZED  No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  0)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
  ---------------------------------------------------------------
   During geometry optimization, the same linked and unlinked
   operators are used.
  ---------------------------------------------------------------
****************************
        SINGLET STATE
****************************
================================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A'    CONVERGED
================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
================================================================
================================================================
```

```
  STEP #SAC#  Solution of SAC equation
================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*******************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*******************************************
HF ENERGY     =    -137.791956 (AU)
SAC-NV  ENERGY=      -0.280551 (AU)
TOTAL ENERGY  =    -138.072507 (AU)
SAC-NV  coefficients (|C|>=0.03)
*SINGLE EXCITATION
       6    9      0.05688
*DOUBLE EXCITATION
       8    9    8    9     -0.08055         8    9    7    9      0.05853
       8   13    8    9      0.05672         6   17    6    9     -0.05550
       8    9    4    9     -0.04890         6   17    5   18     -0.04578
       8   23    8    9     -0.04413         7    9    4    9      0.03895
       8   14    8   12     -0.03894         6   17    6   17     -0.03881
       6    9    6    9     -0.03795         8   14    7   14      0.03422
       6   17    4   16     -0.03387         8   15    8   10     -0.03217
       7   14    6    9     -0.03113         6    9    4   15      0.03096
       8   11    8   10      0.03018         8   11    8   11     -0.03005
Hartree-Fock configuration   1.00000
================================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
================================================================
Energy gradient for SINGLET STATE A'   0-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-NV)=   -0.2805509939 Total energy=      -138.0725073821
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-NV density.
Start back-transformation.
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     595
Number of TU pair in the last loop  =     595
Second-half back-transformation finished.
Solve CP equations for MOD among active MOs.
```

SAC-CI result at the updated geometry. The total energy is decreasing compared with that at the last geometry (-138.072503 au)

```
Max orbital gradient: YijMax=  0.000940 YabMax=  0.000691
DoAtom=TTT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      997720.
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
    1 vectors were produced by pass  8.
    1 vectors were produced by pass  9.
    1 vectors were produced by pass 10.
Inv2:  IOpt= 1 Iter= 1 AM= 3.44D-16 Conv= 1.00D-12.
Inverted reduced A of dimension   11 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          6           0.000410196    0.000000000   -0.000406720
   2          9          -0.001067476    0.000000000   -0.000397162
   3          1           0.000657280    0.000000000    0.000803882
-------------------------------------------------------------------
Cartesian Forces:  Max     0.001067476 RMS     0.000548652

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Berny optimization.
Internal  Forces:  Max     0.000011643 RMS     0.000007905
Search for a local minimum.
Step number   4 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using D2CorX and points  1  2  3  4
Trust test= 1.01D+00 RLast= 4.74D-03 DXMaxT set to 3.00D-01
The second derivative matrix:
                         R1        R2        A1
          R1           0.51224
          R2           0.02689   0.30207
          A1           0.07623  -0.00005   0.35499
    Eigenvalues ---    0.29591   0.32771   0.54568
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.00640.
```

Energy gradient in cartesian coordinate calculated at the updated geometry.

```
Iteration  1 RMS(Cart)=  0.00001775 RMS(Int)=  0.00000000
Iteration  2 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.49743   0.00000   0.00001  -0.00002  -0.00001   2.49742
   R2        2.12856  -0.00001  -0.00002  -0.00001  -0.00004   2.12852
   A1        1.78283   0.00001   0.00001   0.00001   0.00002   1.78285
        Item               Value     Threshold  Converged?
Maximum Force            0.000012     0.000450     YES
RMS     Force            0.000008     0.000300     YES
Maximum Displacement     0.000024     0.001800     YES
RMS     Displacement     0.000018     0.001200     YES
Predicted change in Energy=-2.976457D-10
Optimization completed.
   -- Stationary point found.
                           ----------------------------
                           !   Optimized Parameters   !
                           ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.3216         -DE/DX =    0.0                 !
! R2    R(1,3)                  1.1264         -DE/DX =    0.0                 !
! A1    A(2,1,3)              102.1486         -DE/DX =    0.0                 !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6          0        -0.002725    0.000000   -0.015256
   2          9          0         0.010415    0.000000    1.306261
   3          1          0         1.096024    0.000000   -0.263239
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3
    1  C    0.000000
    2  F    1.321582   0.000000
    3  H    1.126386   1.908370   0.000000
Stoichiometry    CHF
Framework group  CS[SG(CHF)]
Deg. of freedom     3
Full point group                 CS      NOp   2
Largest Abelian subgroup         CS      NOp   2
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
```

Energy gradient and displacements satisfy convergence criteria.

```
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6           0        0.068823    0.728575    0.000000
   2          9           0        0.068823   -0.593008    0.000000
   3          1           0       -1.032338    0.965621    0.000000
---------------------------------------------------------------------
Rotational constants (GHZ):    465.8491572     36.0620779     33.4710352

*********************************************************************

          Population analysis using the SCF density.

*********************************************************************

Orbital symmetries:
      Occupied  (A') (A') (A') (A') (A') (A″) (A') (A')
      Virtual   (A″) (A') (A') (A') (A″) (A') (A') (A') (A″) (A')
                (A') (A') (A″) (A') (A″) (A') (A') (A″) (A') (A″)
                (A') (A') (A') (A') (A') (A')
The electronic state is 1-A'.
Alpha  occ. eigenvalues --  -26.34985 -11.37643  -1.67116  -0.92436  -0.75787
Alpha  occ. eigenvalues --   -0.70734  -0.66448  -0.41052
Alpha virt. eigenvalues --    0.06797   0.25439   0.32862   0.42316   0.49093
Alpha virt. eigenvalues --    0.62796   0.66131   1.01685   1.11480   1.12317
Alpha virt. eigenvalues --    1.20333   1.42011   1.74541   1.76146   1.77056
Alpha virt. eigenvalues --    2.05629   2.31241   2.36072   2.47125   2.83617
Alpha virt. eigenvalues --    2.83783   3.20042   4.01888   4.38570  27.37359
Alpha virt. eigenvalues --   56.52152
         Condensed to atoms (all electrons):
             1          2          3
    1  C    5.400633   0.223622   0.281394
    2  F    0.223622   9.040547  -0.046613
    3  H    0.281394  -0.046613   0.642014
Mulliken atomic charges:
             1
    1  C    0.094351
    2  F   -0.217556
    3  H    0.123205
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  C    0.217556
    2  F   -0.217556
    3  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    55.6705
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
```

```
   X=    -1.5749    Y=     0.2392    Z=     0.0000  Tot=     1.5930
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=   -11.7136   YY=   -12.6755   ZZ=   -10.0513
  XY=    -1.8537   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -0.2335   YY=    -1.1954   ZZ=     1.4289
  XY=    -1.8537   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=    -1.6996  YYY=    -8.6042  ZZZ=     0.0000  XYY=    -2.4690
 XXY=    -2.8792  XXZ=     0.0000  XZZ=    -0.3342  YZZ=    -1.5594
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=   -15.9341 YYYY=   -45.5514 ZZZZ=    -7.4595 XXXY=    -0.3228
XXXZ=     0.0000 YYYX=    -1.7828 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=   -10.7197 XXZZ=    -4.0435 YYZZ=    -8.2020
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.1375
N-N= 2.693668490679D+01 E-N=-3.814339160477D+02  KE= 1.377006737460D+02
Symmetry A'   KE= 1.318265750304D+02
Symmetry A"   KE= 5.874098715628D+00
Final structure in terms of initial Z-matrix:
C
F,1,FC
H,1,HC,2,HCF
     Variables:
FC=1.32158207
HC=1.12638571
HCF=102.148632

Test job not archived.
1¥1¥GINC-MIRAI86¥FOpt¥RSACCI¥D95(d)¥C1H1F1¥MASAHIRO¥03-Aug-2004¥0¥¥# S
AC-CI(SACONLY, TARGETSTATE=(SPINSTATE=SINGLET,SYMMETRY=1,ROOT=0)) /D95
(D) OPT TEST¥¥Gaussian Test Job 638 (Part 2): Geometry optimization of
 the SAC ground state of HCF. Initial geometry is the experimental one
. MacroIter=1 (default).¥¥0,1¥C,-0.0760629773,0.,-0.7278542531¥F,-0.06
29231291,0.,0.5936624943¥H,1.0226860252,0.,-0.97583693¥¥Version=AI64T-
G03RevC.02¥State=1-A'¥HF=-137.7919564¥RMSD=9.002e-09¥RMSF=5.487e-04¥Di
pole=0.5766617,0.,-0.0075208¥PG=CS [SG(C1H1F1)]¥¥@


If your ship doesn't come in, swim out to it!
                          -- Jonathan Winters
Job cpu time:  0 days  0 hours  7 minutes 17.9 seconds.
File lengths (MBytes):  RWF=    479 Int=      0 D2E=      0 Chk=     10 Scr=     19
Normal termination of Gaussian 03 at Tue Aug  3 13:34:22 2004.
```

Output 647

```
Entering Gaussian System, Link 0=/work/g03.C02/g03/g03
```

```
Initial command:
/work/g03.C02/g03/l1.exe /work/g03.C02/inputs/Gau-185105.inp -scrdir=/work/g03.C02/inputs/
Entering Link 1 = /work/g03.C02/g03/l1.exe PID=    185104.

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C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

*****************************************
Gaussian 03:  AI64T-G03RevC.02 12-Jun-2004
                 3-Aug-2004
*****************************************
%mem=12mw
---------------------------------------------------------------------------
# SAC-CI(Singlet=(NState=(0,1,0,0)), TargetState=(SpinState=Singlet,Sy
mmetry=2,Root=1), General-R) /D95** Opt CPHF=Canonical test
---------------------------------------------------------------------------

Warning:  CPHF=MOD not CPHF=Canonical is strongly recommended with GSUM.
1/18=20,38=1/1,3;
2/9=110,17=6,18=5,40=1/2;
3/5=8,7=101,11=9,16=1,25=1,30=1,36=2/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=5,9=30000,10=1,40=1,42=1/1,4;
9/15=1/23;
11/28=-14,29=200,42=3,46=1/11;
10/5=5/2;
6/7=2,8=2,9=2,10=2/1;
7/12=7/1,2,3,16;
1/18=20/3(1);
99//99;
```

List of keywords given in the Gaussian input. This is SAC-CI general-R calculation for the geometry of two-electron excited state (1^1A_2 state of BH).

```
2/9=110/2;
3/5=8,7=101,11=9,16=1,25=1,30=1,36=2/1,2,3;
4/5=5,16=3/1;
5/5=2,38=5/2;
8/6=5,9=30000,10=1,40=1,42=1/1,4;
9/15=1/23;
11/28=-14,29=200,42=3,46=1/11;
10/5=5/2;
7/12=7/1,2,3,16;
1/18=20/3(-9);
2/9=110/2;
6/7=2,8=2,9=2,10=2/1;
99//99;
-----------------------------------------------------------------------
Gaussian Test Job 647 (Part 1): SAC-CI general-R geometry optimization
 calculation for the singlet Delta excited state of BH with D95**. Ful
l-valence active MOs are used (FC; default). Initial geometry is the e
xperimental one. Since singlet delta excited state is two-electron exc
ited state, general-R method is more reliable than the SD-R method. So
, for comparison, SAC-CI SD-R calculation is also done below for compa
rison. The results are summarized in Part I-L of the SAC-CI Guide.
-----------------------------------------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
B
H                    1    BH
      Variables:
 BH                    1.1963


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                         ----------------------------
                         !    Initial Parameters    !
                         ! (Angstroms and Degrees)  !
--------------------------                          --------------------------
! Name  Definition              Value          Derivative Info.                !
-----------------------------------------------------------------------------
! R1    R(1,2)                  1.1963         estimate D2E/DX2                !
-----------------------------------------------------------------------------
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
```

Variable (B-H distance) to be optimized, ant its initial value.

```
---------------------------------------------------------------------
   1          5             0        0.000000    0.000000    0.000000
   2          1             0        0.000000    0.000000    1.196300
---------------------------------------------------------------------
Stoichiometry    BH
Framework group  C*V[C*(HB)]
Deg. of freedom     1
Full point group                 C*V     NOp   4
Largest Abelian subgroup         C2V     NOp   4
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5             0        0.000000    0.000000    0.199383
   2          1             0        0.000000    0.000000   -0.996917
---------------------------------------------------------------------
Rotational constants (GHZ):      0.0000000    382.4658857    382.4658857
Standard basis: D95(d,p) (6D, 7F)
There are    12 symmetry adapted basis functions of A1  symmetry.
There are     1 symmetry adapted basis functions of A2  symmetry.
There are     4 symmetry adapted basis functions of B1  symmetry.
There are     4 symmetry adapted basis functions of B2  symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   21 basis functions,    37 primitive gaussians,    21 cartesian basis functions
    3 alpha electrons        3 beta electrons
      nuclear repulsion energy         2.2117245185 Hartrees.
NAtoms=    2 NActive=    2 NUniq=    2 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    21 RedAO= T  NBF=    12     1     4     4
NBsUse=    21 1.00D-06 NBFU=    12     1     4     4
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 7.01D-02 ExpMax= 2.79D+03 ExpMxC= 4.19D+02 IAcc=2 IRadAn=         4 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Initial guess orbital symmetries:
      Occupied  (SG) (SG) (SG)
      Virtual   (PI) (PI) (SG) (PI) (PI) (SG) (SG) (SG) (PI) (PI)
                (DLTA) (DLTA) (SG) (PI) (PI) (SG) (SG) (SG)
The electronic state of the initial guess is 1-SG.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=      871060.
SCF Done:  E(RHF) =  -25.1233368036     A.U. after    8 cycles
```

```
            Convg  =    0.5126D-08             -V/T =  1.9995
            S**2   =   0.0000
Perform MO ordering.
ExpMin= 7.01D-02 ExpMax= 2.79D+03 ExpMxC= 4.19D+02 IAcc=3 IRadAn=        5 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=        5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     2    20
NBasis=    21 NAE=     3 NBE=     3 NFC=     1 NFV=     1
NROrb=     19 NOA=     2 NOB=     2 NVA=    17 NVB=    17
--------------------------------------------------------------------------
##########################################################################
--------------------------------------------------------------------------
              SAC/SAC-CI Program Combined with GAUSSIAN
                            for Calculating
        Ground, Excited, Ionized, and Electron-Attached States
                                and
            Singlet, Doublet, Triplet, Quartet, Quintet,
                  Sextet, and Septet Spin States
                                and
                 Their Analytical Energy Gradients
                        coded originally by
                         Hiroshi Nakatsuji
                          and extended by
 H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa,
      M. Ishida, T. Nakajima, Y. Honda, O. Kitao, and H. Nakai
                                at
                 Department of Hydrocarbon Chemistry,
                Division of Molecular Engineering, and
     Department of Synthetic Chemistry & Biological Chemistry,
                  Graduate School of Engineering,
                         Kyoto University,
                       Kyoto 606-8501, Japan
--------------------------------------------------------------------------
##########################################################################
--------------------------------------------------------------------------
No. of INTEGRALS =      5257 NBLK =         3 KOUNT =       457
  Calculate the SAC-CI general-R gradients. IGROpt=   1
******************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 0
******************************************************************************
===============================================================
  STEP #PRES#  Generation of Linked Operators and Selection
===============================================================
== States to be calculated ==
           A1   A2   B1   B2
SINGLET    Yes  No   No   No
TRIPLET    No   No   No   No
IONIZED    No   No   No   No
ANIONIZED  No   No   No   No
```

Beginning of the SAC-CI part of the program

```
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  0,  0,  0)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
****************************
        SINGLET STATE
****************************
-------------------------------------------------------------
LINKED OPERATORS FOR SAC:    SYMMETRY = A1  GROUND STATE
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            16         211          227
    AFTER             16         170          187
=============================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
=============================================================
=============================================================
  STEP #DIAGCI#  Solution of SDCI
=============================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A1    CONVERGED
=============================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
=============================================================
Threshold for S2 operator (CThreULS2G) 0.500D-02
=============================================================
  STEP #SAC#  Solution of SAC equation
=============================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*******************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*******************************************
HF ENERGY     =     -25.123337 (AU)
SAC-NV  ENERGY=      -0.081563 (AU)
TOTAL ENERGY  =     -25.204899 (AU)
*****************************************************************************
    SAC-CI GENERAL-R  Geometry optimization.  IStep= 0
*****************************************************************************
SINGLET STATE
  Number of States  Singlet       =(  0  1  0  0)
  Perturbation selection with reference state
```

Perturbation selection for the ground state. Number of single and double excitation operators in SAC w.f. before and after the selection.

Result of SAC calculation. Hartree-Fock (HF) energy, SAC-NV energy (correlation energy obtained with the SAC method).

```
   Threshold of perturbation selection of linked operator # LevelThree #
    EThreR2(E) (Lambda_E)=  0.100D-06(au)
   Spin functions of selected operators may be incomplete.
  Calculate SAC-CI general-R gradients. IStep =   0
  Target State =   1 Target Symmetry =   2
  MOs for active space:   2  17     MOs for small active space:   2  17
  Spin state        Sol. of Reference-CI       Sol. of A-CI and B-CI     MaxR
  Singlet            0  1  0  0                 0  1  0  0               3
Singlet
  B-operator: SDCI for reference-CI with small active space
  Generate all the higher-order excitation operators
  Skip higher-order unlinked terms
*********************************************
              SINGLET STATE
*********************************************
STEP #MEGI# : Calculation of integrals for REFERENCE-CI ... DONE
STEP #DAS#  : Direct diagonalization for reference-CI ... Done
=====================================================================
  STEP #GHPRES#  Generation of A-CI, B-CI operators and selection
=====================================================================
*Reference configurations for Singlet       A2
    1:   3   5   3   4                2:   3   7   3   5
    3:   3   8   3   4                4:   3   5   2   4
    5:   3   4   2   5
  Square norm of reference state with above configurations:
   1: 0.97806
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = A2  EXCITED STATE
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            2          96           98
    AFTER             2          64           66
STEP #MEGI# : Calculation of integrals for SDCI ... DONE
Solution for Singlet   A2    CONVERGED
STEP #SCIV# :   Iterative diagonalization for SD-CI ... Done
=====================================================================
  STEP #EGOP#  Exponential generation of higher-operators
=====================================================================
All the higher-order excitation operators are generated.
Perturbation selection with reference states
 Threshold for perturbation selection, EThreEgR (Lambda_E)   0.10D-05(AU)
== Estimation of full dimensions ==
 3-Ples:      3264   4-Ples:      6936
-------------------------------------------------------------------------
Singlet        A2     Number of linked operators for SAC-CI general-R
 TOTAL:    246  1-PLE:      2  2-PLE:     64  3-PLE:    180  4-PLE:      0
               5-PLE:      0  6-PLE:      0
=====================================================================
  STEP #MEGI#  Calculates CI matrix elements
=====================================================================
```

Up to triple excitation operators are included in the SAC-CI general-R wave function.

Number of the linked operators for single- and double- excitation operators in SAC-CI w.f. before and after the perturbation selection

Exponential generation of the excitation operators higher than doubles. To determine the linked operator, the second-order energy is evaluated for the generated operators with the threshold EThreEgR.

Number of the linked operators for single, double, and triple excitation operators in SAC-CI w.f. after the perturbation selection.

```
=============================================================
  STEP #MEGI#  Calculates unlinked integrals
=============================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
=============================================================
  STEP #SCIV#  Iterative diagonalization OF SAC-CI-V
=============================================================
Threshold for density convergence (DConvDiag) .10
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A2    CONVERGED
**********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
**********************************************
**********************************************
Singlet        A2      ************************
###   1-st  ###           ---   1st state in this spin                  y ---
    This state is being used for optimizations.
    Total energy       in au =     -24.979507
    Correlation energy in au =       0.143830
    Excitation energy  in au =       0.22539      in eV =       6.133239
  *SINGLE EXCITATION
       3   15       -0.04543
  *DOUBLE EXCITATION
       3    5    3    4   0.88642         3    7    3    5   0.28910
       3    8    3    4   0.28757         3    5    2    4  -0.11501
       3    4    2    5  -0.11140         2    5    2    4  -0.09094
       3    5    2    7  -0.04586         3    4    2    8  -0.04402
       3   13    2    4   0.03262         3   12    2    5   0.03248
       2    7    2    5  -0.03013
  *TRIPLE EXCITATION
       3   11    2    5    2    4  -0.04289
       3   14    3    5    2    4  -0.03958
       3    6    2    5    2    4   0.03818
=============================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
=============================================================
Energy gradient for SINGLET STATE        A2   1-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-CI-GR-V)=    0.1438297991 Total energy=       -24.9795070045
Z-vector iteration Converged
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-CI-V / SAC-NV density.
Gamma from SAC-CI General-R- V(singlet). Symmetry  2
With HF: IHF=         1 NDTEX=       246
```

SAC-CI result for singlet state. This state is the target state of the geometry oprimization. Total energy, correlation energy (HF energy as the reference), excitation energy (SAC total energy as the reference), and the SAC-CI coefficients are shown. The 1^1A_1 state is characterized as two-electron excitation from 3-rd MO to 5- and 4-th MOs, and its coefficients is 0.89. The excitation energy is 6.13 eV.

```
Start back-transformation.
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     231
Number of TU pair in the last loop  =     231
Second-half back-transformation finished.
Use canonical orbitals for SAC/SAC-CI optimization.
Tollerance for orbital energy difference is  0.100D-08
Warning: This can cause divergence of gradients.
Max orbital gradient: YijMax=  0.000222 YabMax=  0.001449
DoAtom=TT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      847150.
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
Inv2:  IOpt= 1 Iter= 1 AM= 3.22D-16 Conv= 1.00D-12.
Inverted reduced A of dimension    8 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.

**********************************************************************

           Population analysis using the SCF density.

**********************************************************************

Orbital symmetries:
      Occupied  (SG) (SG) (SG)
      Virtual   (PI) (PI) (SG) (PI) (PI) (SG) (SG) (SG) (PI) (PI)
                (DLTA) (DLTA) (SG) (PI) (PI) (SG) (SG) (SG)
The electronic state is 1-SG.
Alpha  occ. eigenvalues --   -7.68806  -0.65982  -0.34280
Alpha virt. eigenvalues --    0.04885   0.04885   0.22465   0.35251   0.35251
Alpha virt. eigenvalues --    0.41580   0.47365   1.24530   1.59015   1.59015
Alpha virt. eigenvalues --    1.74820   1.74820   2.06748   2.45977   2.45977
Alpha virt. eigenvalues --    3.30089   4.76964  20.46702
         Condensed to atoms (all electrons):
             1          2
    1  B    4.671320   0.299095
    2  H    0.299095   0.730491
```

```
Mulliken atomic charges:
             1
    1  B    0.029585
    2  H   -0.029585
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  B    0.000000
    2  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    21.8244
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     0.0000    Y=     0.0000    Z=    -2.0878  Tot=     2.0878
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -6.5054   YY=    -6.5054   ZZ=   -10.6155
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=     1.3700   YY=     1.3700   ZZ=    -2.7401
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=     0.0000  YYY=     0.0000  ZZZ=    -6.5665  XYY=     0.0000
 XXY=     0.0000  XXZ=    -1.6113  XZZ=     0.0000  YZZ=     0.0000
 YYZ=    -1.6113  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=    -8.6284 YYYY=    -8.6284 ZZZZ=   -27.2484 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=    -2.8761 XXZZ=    -5.9830 YYZZ=    -5.9830
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 2.211724518515D+00 E-N=-6.242547858997D+01  KE= 2.513671486323D+01
Symmetry A1   KE= 2.513671486323D+01
Symmetry A2   KE= 0.000000000000D+00
Symmetry B1   KE= 0.000000000000D+00
Symmetry B2   KE= 0.000000000000D+00
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          5           0.000000000    0.000000000   -0.001648656
   2          1           0.000000000    0.000000000    0.001648656
-------------------------------------------------------------------
Cartesian Forces:  Max     0.001648656 RMS     0.000951852

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.001648656 RMS     0.001648656
Search for a local minimum.
Step number   1 out of a maximum of  20
```

Energy gradient in cartesian coordinate calculated at the initial geometry.

```
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- first step.
The second derivative matrix:
                          R1
          R1           0.24937
    Eigenvalues ---    0.24937
RFO step:  Lambda=-1.08991060D-05.
Linear search not attempted -- first point.
Iteration  1 RMS(Cart)=  0.00467462 RMS(Int)=  0.00000000
Iteration  2 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.26068   0.00165   0.00000   0.00661   0.00661   2.26729
        Item               Value     Threshold  Converged?
Maximum Force            0.001649     0.000450     NO
RMS     Force            0.001649     0.000300     NO
Maximum Displacement     0.003305     0.001800     NO
RMS     Displacement     0.004675     0.001200     NO
Predicted change in Energy=-5.449791D-06
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5            0        0.000000    0.000000   -0.001749
   2          1            0        0.000000    0.000000    1.198049
---------------------------------------------------------------------
Stoichiometry    BH
Framework group  C*V[C*(HB)]
Deg. of freedom     1
Full point group                 C*V     NOp   4
Largest Abelian subgroup         C2V     NOp   4
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5            0        0.000000    0.000000    0.199966
   2          1            0        0.000000    0.000000   -0.999832
---------------------------------------------------------------------
Rotational constants (GHZ):      0.0000000    380.2387698    380.2387698
Standard basis: D95(d,p) (6D, 7F)
There are    12 symmetry adapted basis functions of A1  symmetry.
There are     1 symmetry adapted basis functions of A2  symmetry.
There are     4 symmetry adapted basis functions of B1  symmetry.
There are     4 symmetry adapted basis functions of B2  symmetry.
```

Energy gradient and displacements do not satisfy convergence criteria.

The second geometry to be calculated.

```
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   21 basis functions,    37 primitive gaussians,    21 cartesian basis functions
    3 alpha electrons        3 beta electrons
      nuclear repulsion energy         2.2052756314 Hartrees.
NAtoms=    2 NActive=    2 NUniq=    2 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    21 RedAO= T  NBF=    12     1     4     4
NBsUse=    21 1.00D-06 NBFU=    12     1     4     4
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (SG) (SG) (SG)
      Virtual   (PI) (PI) (SG) (PI) (PI) (SG) (SG) (SG) (PI) (PI)
                (DLTA) (DLTA) (SG) (PI) (PI) (SG) (SG) (SG)
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=      871060.
SCF Done:  E(RHF) =  -25.1234383984     A.U. after    7 cycles
            Convg  =    0.1032D-08             -V/T =  1.9996
            S**2   =   0.0000
Perform MO ordering.
Number of Electrons          6
Spin Multiplicity            1
Number of Occupieds          3
Number of Molecular Charge   0
Use orbital energies in MO ordering; INotEig=    0.
Use dipole moments in MO ordering; IFlagDP=    1.
Use second moments in MO ordering; IFlagSM=    1.
ExpMin= 7.01D-02 ExpMax= 2.79D+03 ExpMxC= 4.19D+02 IAcc=3 IRadAn=         5 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=         5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     2    20
NBasis=    21 NAE=     3 NBE=     3 NFC=     1 NFV=     1
NROrb=     19 NOA=     2 NOB=     2 NVA=    17 NVB=    17
No. of INTEGRALS =      5257 NBLK =         3 KOUNT =       457
  Calculate the SAC-CI general-R gradients. IGROpt=   1
*****************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 1
*****************************************************************************
==============================================================
  STEP #PRES#  Generation of Linked Operators and Selection
==============================================================
== States to be calculated ==
           A1   A2   B1   B2
SINGLET    Yes  No   No   No
TRIPLET    No   No   No   No
```

```
IONIZED    No   No   No   No
ANIONIZED  No   No   No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  0,  0,  0)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
  ------------------------------------------------------------
   During geometry optimization, the same linked and unlinked
   operators are used.
  ------------------------------------------------------------
****************************
        SINGLET STATE
****************************
================================================================
  STEP #CIMX#  CI matrix elements         ### SINGLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A1    CONVERGED
================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
================================================================
================================================================
  STEP #SAC#  Solution of SAC equation
================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*******************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*******************************************
HF ENERGY     =     -25.123438 (AU)
SAC-NV  ENERGY=      -0.081587 (AU)
TOTAL ENERGY  =     -25.205026 (AU)
*******************************************************************************
    SAC-CI GENERAL-R  Geometry optimization. IStep= 1
*******************************************************************************
SINGLET STATE
  Number of States  Singlet       =(  0  1  0  0)
  Perturbation selection with reference state
```

```
   Threshold of perturbation selection of linked operator # LevelThree #
    EThreR2(E) (Lambda_E)=  0.100D-06(au)
   Spin functions of selected operators may be incomplete.
  Calculate SAC-CI general-R gradients. IStep =   1
  Target State =   1 Target Symmetry =   2
  MOs for active space:   2  17     MOs for small active space:   2  17
  Spin state        Sol. of Reference-CI       Sol. of A-CI and B-CI     MaxR
  Singlet            0  1  0  0                 0  1  0  0               3
Singlet
  B-operator: SDCI for reference-CI with small active space
  Generate all the higher-order excitation operators
  Skip higher-order unlinked terms
STEP #MEGI# : Calculation of integrals for REFERENCE-CI ... DONE
STEP #DAS#  : Direct diagonalization for reference-CI ... Done
=====================================================================
  STEP #GHPRES#  Generation of A-CI, B-CI operators and selection
=====================================================================
STEP #MEGI# : Calculation of integrals for SDCI ... DONE
Solution for Singlet   A2    CONVERGED
STEP #SCIV# :   Iterative diagonalization for SD-CI ... Done
=================================================================
  STEP #MEGI#  Calculates CI matrix elements
=================================================================
=================================================================
  STEP #MEGI#  Calculates unlinked integrals
=================================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
=================================================================
  STEP #SCIV#  Iterative diagonalization OF SAC-CI-V
=================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A2    CONVERGED
**********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
**********************************************
*****************************************************************************
Singlet        A2      ******************************************************
###   1-st  ###           ---   1st state in this spin multiplicity ---
    This state is being used for optimizations.
    Total energy       in au =     -24.979512
    Correlation energy in au =       0.143926
    Excitation energy  in au =       0.225513    in eV =       6.136534
  *SINGLE EXCITATION
       3   15        0.04544
  *DOUBLE EXCITATION
       3    5    3    4  -0.88664         3    7    3    5  -0.28886
       3    8    3    4  -0.28732         3    5    2    4   0.11407
```

SAC-CI result at the updated geometry. The total energy is decreasing compared with that at the last geometry (-24.979507 au)

```
      3    4    2    5   0.11045         2    5    2    4   0.09155
      3    5    2    7   0.04539         3    4    2    8   0.04356
      3   13    2    4  -0.03263         3   12    2    5  -0.03249
      2    7    2    5   0.03030         2    8    2    4   0.03004
  *TRIPLE EXCITATION
      3   11    2    5    2    4   0.04291
      3   14    3    5    2    4   0.03959
      3    6    2    5    2    4  -0.03836
================================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
================================================================
Energy gradient for SINGLET STATE        A2   1-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-CI-GR-V)=    0.1439261082 Total energy=       -24.9795122902
Z-vector iteration Converged
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-CI-V / SAC-NV density.
Gamma from SAC-CI General-R- V(singlet). Symmetry  2
With HF: IHF=         1 NDTEX=       246
Start back-transformation.
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     231
Number of TU pair in the last loop  =     231
Second-half back-transformation finished.
Use canonical orbitals for SAC/SAC-CI optimization.
Tollerance for orbital energy difference is  0.100D-08
Warning: This can cause divergence of gradients.
Max orbital gradient: YijMax=  0.000231 YabMax=  0.001445
DoAtom=TT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      847150.
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
Inv2:  IOpt= 1 Iter= 1 AM= 2.95D-16 Conv= 1.00D-12.
```

```
Inverted reduced A of dimension    8 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          5           0.000000000    0.000000000    0.000042305
   2          1           0.000000000    0.000000000   -0.000042305
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000042305 RMS     0.000024425

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.000042305 RMS     0.000042305
Search for a local minimum.
Step number   2 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using D2CorX and points  1  2
Trust test= 9.70D-01 RLast= 6.61D-03 DXMaxT set to 3.00D-01
The second derivative matrix:
                          R1
          R1           0.25578
    Eigenvalues ---    0.25578
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.02533.
Iteration  1 RMS(Cart)=  0.00011843 RMS(Int)=  0.00000000
Iteration  2 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.26729  -0.00004  -0.00017   0.00000  -0.00017   2.26712
        Item               Value     Threshold  Converged?
Maximum Force            0.000042     0.000450     YES
RMS     Force            0.000042     0.000300     YES
Maximum Displacement     0.000084     0.001800     YES
RMS     Displacement     0.000118     0.001200     YES
Predicted change in Energy=-3.497867D-09
Optimization completed.
   -- Stationary point found.
                           ----------------------------
                           !   Optimized Parameters   !
                           ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
-----------------------------------------------------------------------------
! R1    R(1,2)                  1.1998         -DE/DX =    0.0                 !
-----------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
```

Energy gradient in cartesian coordinate calculated at the updated geometry.

Energy gradient and displacements satisfy convergence criteria.

Optimized B-H distance

```
                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5            0        0.000000    0.000000   -0.001749
   2          1            0        0.000000    0.000000    1.198049
---------------------------------------------------------------------
Stoichiometry    BH
Framework group  C*V[C*(HB)]
Deg. of freedom     1
Full point group                 C*V     NOp   4
Largest Abelian subgroup         C2V     NOp   4
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5            0        0.000000    0.000000    0.199966
   2          1            0        0.000000    0.000000   -0.999832
---------------------------------------------------------------------
Rotational constants (GHZ):      0.0000000    380.2387698    380.2387698

*********************************************************************

           Population analysis using the SCF density.

*********************************************************************

Orbital symmetries:
      Occupied  (SG) (SG) (SG)
      Virtual   (PI) (PI) (SG) (PI) (PI) (SG) (SG) (SG) (PI) (PI)
                (DLTA) (DLTA) (SG) (PI) (PI) (SG) (SG) (SG)
The electronic state is 1-SG.
Alpha  occ. eigenvalues --   -7.68845  -0.65888  -0.34292
Alpha virt. eigenvalues --    0.04879   0.04879   0.22494   0.35243   0.35243
Alpha virt. eigenvalues --    0.41417   0.47358   1.24503   1.59049   1.59049
Alpha virt. eigenvalues --    1.74805   1.74805   2.06287   2.45670   2.45670
Alpha virt. eigenvalues --    3.29485   4.76950  20.46680
         Condensed to atoms (all electrons):
             1          2
    1  B    4.670256   0.298848
    2  H    0.298848   0.732049
Mulliken atomic charges:
             1
    1  B    0.030896
    2  H   -0.030896
Sum of Mulliken charges=   0.00000
```

```
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  B    0.000000
    2  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    21.8596
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     0.0000    Y=     0.0000    Z=    -2.0772  Tot=     2.0772
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -6.5087   YY=    -6.5087   ZZ=   -10.6226
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=     1.3713   YY=     1.3713   ZZ=    -2.7426
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=     0.0000  YYY=     0.0000  ZZZ=    -6.5468  XYY=     0.0000
 XXY=     0.0000  XXZ=    -1.6039  XZZ=     0.0000  YZZ=     0.0000
 YYZ=    -1.6039  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=    -8.6322 YYYY=    -8.6322 ZZZZ=   -27.3257 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=    -2.8774 XXZZ=    -5.9963 YYZZ=    -5.9963
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 2.205275631355D+00 E-N=-6.241038535938D+01  KE= 2.513345968012D+01
Symmetry A1   KE= 2.513345968012D+01
Symmetry A2   KE=-4.815442214459D-51
Symmetry B1   KE= 0.000000000000D+00
Symmetry B2   KE= 0.000000000000D+00
Final structure in terms of initial Z-matrix:
B
H,1,BH
     Variables:
BH=1.19979834

Test job not archived.
1¥1¥GINC-MIRAI86¥FOpt¥RSACCI¥D95(d,p)¥B1H1¥MASAHIRO¥03-Aug-2004¥0¥¥# S
AC-CI(SINGLET=(NSTATE=(0,1,0,0)), TARGETSTATE=(SPINSTATE=SINGLET,SYMME
TRY=2,ROOT=1), GENERAL-R) /D95** OPT CPHF=CANONICAL TEST¥¥Gaussian Tes
t Job 647 (Part 1): SAC-CI general-R geometry optimization calculation
 for the singlet Delta excited state of BH with D95**. Full-valence ac
tive MOs are used (FC; default). Initial geometry is the experimental
one. Since singlet delta excited state is two-electron excited state,
general-R method is more reliable than the SD-R method. So, for compar
ison, SAC-CI SD-R calculation is also done below for comparison. The r
esults are summarized in Part I-L of the SAC-CI Guide.¥¥0,1¥B,0.,0.,-0
.19996639¥H,0.,0.,0.9998319499¥¥Version=AI64T-G03RevC.02¥State=1-SG¥HF
=-25.1234384¥RMSD=1.032e-09¥RMSF=2.442e-05¥Dipole=0.,0.,-0.2168712¥PG=
C*V [C*(H1B1)]¥¥@
```

```
FAULTILY FAULTLESS, ICILY REGULAR, SPLENDIDLY NULL...
          MAUDE BY TENNYSON
Job cpu time:  0 days  0 hours  0 minutes 15.6 seconds.
File lengths (MBytes):  RWF=    115 Int=      0 D2E=      0 Chk=     10 Scr=     28
Normal termination of Gaussian 03 at Tue Aug  3 13:36:23 2004.
Initial command:
/work/g03.C02/g03/l1.exe /work/g03.C02/inputs/Gau-185105.inp -scrdir=/work/g03.C02/inputs/
Entering Link 1 = /work/g03.C02/g03/l1.exe PID=    185110.

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I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

******************************************
Gaussian 03:  AI64T-G03RevC.02 12-Jun-2004
                3-Aug-2004
******************************************
%mem=12mw
--------------------------------------------------------------------------------
# SAC-CI(Singlet=(NState=(0,1,0,0),MaxR=2), TargetState=(SpinState=Sin
glet,Symmetry=2,Root=1), General-R) /D95** Opt CPHF=Canonical test
--------------------------------------------------------------------------------

Warning:  CPHF=MOD not CPHF=Canonical is strongly recommended with GSUM.
1/18=20,38=1/1,3;
2/9=110,17=6,18=5,40=1/2;
3/5=8,7=101,11=9,16=1,25=1,30=1,36=2/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=5,9=30000,10=1,40=1,42=1/1,4;
```

List of keywords given in the Gaussian input. This is SAC-CI SD-R (MaxR=2) calculation for the geometry of 1^1A_2 state of BH. The result of the calculation is compared with that by the general-R (See section I-L for summary)

```
9/15=1/23;
11/28=-14,29=200,42=3,46=1/11;
10/5=5/2;
6/7=2,8=2,9=2,10=2/1;
7/12=7/1,2,3,16;
1/18=20/3(1);
99//99;
2/9=110/2;
3/5=8,7=101,11=9,16=1,25=1,30=1,36=2/1,2,3;
4/5=5,16=3/1;
5/5=2,38=5/2;
8/6=5,9=30000,10=1,40=1,42=1/1,4;
9/15=1/23;
11/28=-14,29=200,42=3,46=1/11;
10/5=5/2;
7/12=7/1,2,3,16;
1/18=20/3(-9);
2/9=110/2;
6/7=2,8=2,9=2,10=2/1;
99//99;
-----------------------------------------------------------------------
Gaussian Test Job 647 (Part 2): SAC-CI SD-R geometry optimization calc
ulation for the singlet Delta excited state of BH with full-valence ac
tive MOs of D95**. Initial geometry is the experimental one.
-----------------------------------------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
B
H                    1    BH
      Variables:
 BH                    1.1963


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                         ----------------------------
                         !    Initial Parameters    !
                         ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.1963         estimate D2E/DX2                !
--------------------------------------------------------------------------------
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
```

Variable (B-H distance) to be optimized, ant its initial value.

```
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5            0        0.000000    0.000000    0.000000
   2          1            0        0.000000    0.000000    1.196300
---------------------------------------------------------------------
Stoichiometry    BH
Framework group  C*V[C*(HB)]
Deg. of freedom     1
Full point group                 C*V     NOp   4
Largest Abelian subgroup         C2V     NOp   4
Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5            0        0.000000    0.000000    0.199383
   2          1            0        0.000000    0.000000   -0.996917
---------------------------------------------------------------------
Rotational constants (GHZ):      0.0000000    382.4658857    382.4658857
Standard basis: D95(d,p) (6D, 7F)
There are    12 symmetry adapted basis functions of A1  symmetry.
There are     1 symmetry adapted basis functions of A2  symmetry.
There are     4 symmetry adapted basis functions of B1  symmetry.
There are     4 symmetry adapted basis functions of B2  symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   21 basis functions,    37 primitive gaussians,    21 cartesian basis functions
    3 alpha electrons        3 beta electrons
      nuclear repulsion energy         2.2117245185 Hartrees.
NAtoms=    2 NActive=    2 NUniq=    2 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    21 RedAO= T  NBF=    12     1     4     4
NBsUse=    21 1.00D-06 NBFU=    12     1     4     4
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 7.01D-02 ExpMax= 2.79D+03 ExpMxC= 4.19D+02 IAcc=2 IRadAn=         4 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Initial guess orbital symmetries:
      Occupied  (SG) (SG) (SG)
      Virtual   (PI) (PI) (SG) (PI) (PI) (SG) (SG) (SG) (PI) (PI)
                (DLTA) (DLTA) (SG) (PI) (PI) (SG) (SG) (SG)
The electronic state of the initial guess is 1-SG.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
```

```
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=      871060.
SCF Done:  E(RHF) =  -25.1233368036     A.U. after    8 cycles
            Convg  =    0.5126D-08             -V/T =  1.9995
            S**2   =   0.0000
Perform MO ordering.
ExpMin= 7.01D-02 ExpMax= 2.79D+03 ExpMxC= 4.19D+02 IAcc=3 IRadAn=        5 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=        5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     2    20
NBasis=    21 NAE=     3 NBE=     3 NFC=     1 NFV=     1
NROrb=     19 NOA=     2 NOB=     2 NVA=    17 NVB=    17
-----------------------------------------------------------------------
#######################################################################
-----------------------------------------------------------------------
              SAC/SAC-CI Program Combined with GAUSSIAN
                            for Calculating
        Ground, Excited, Ionized, and Electron-Attached States
                                and
            Singlet, Doublet, Triplet, Quartet, Quintet,
                  Sextet, and Septet Spin States
                                and
                 Their Analytical Energy Gradients
                        coded originally by
                         Hiroshi Nakatsuji
                          and extended by
 H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa,
      M. Ishida, T. Nakajima, Y. Honda, O. Kitao, and H. Nakai
                                at
                 Department of Hydrocarbon Chemistry,
                Division of Molecular Engineering, and
      Department of Synthetic Chemistry & Biological Chemistry,
                  Graduate School of Engineering,
                         Kyoto University,
                       Kyoto 606-8501, Japan
-----------------------------------------------------------------------
#######################################################################
-----------------------------------------------------------------------
No. of INTEGRALS =      5257 NBLK =         3 KOUNT =       457
  Calculate the SAC-CI general-R gradients. IGROpt=   1
*******************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 0
*******************************************************************************
===============================================================
  STEP #PRES#  Generation of Linked Operators and Selection
===============================================================
== States to be calculated ==
           A1   A2   B1   B2
SINGLET    Yes  No   No   No
```

```
TRIPLET    No   No   No   No
IONIZED    No   No   No   No
ANIONIZED  No   No   No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  0,  0,  0)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
****************************
        SINGLET STATE
****************************
------------------------------------------------------------
LINKED OPERATORS FOR SAC:    SYMMETRY = A1  GROUND STATE
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            16         211          227
    AFTER             16         170          187
==============================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
==============================================================
==============================================================
  STEP #DIAGCI#  Solution of SDCI
==============================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A1    CONVERGED
==============================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
==============================================================
Threshold for S2 operator (CThreULS2G) 0.500D-02
==============================================================
  STEP #SAC#  Solution of SAC equation
==============================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*********************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*********************************************
HF ENERGY     =     -25.123337 (AU)
SAC-NV  ENERGY=      -0.081563 (AU)
TOTAL ENERGY  =     -25.204899 (AU)
*****************************************************************************
    SAC-CI GENERAL-R  Geometry optimization. IStep= 0
*****************************************************************************
```

Number of the linked operators for single- and double- excitation operators in SAC w.f. before and after the perturbation selection

Result of SAC calculation. Hartree-Fock (HF) energy, SAC-NV energy (correlation energy obtained with the SAC method).

```
SINGLET STATE
  Number of States  Singlet       =(  0  1  0  0)
  Perturbation selection with reference state
   Threshold of perturbation selection of linked operator # LevelThree #
    EThreR2(E) (Lambda_E)=  0.100D-06(au)
   Spin functions of selected operators may be incomplete.
  Calculate SAC-CI general-R gradients. IStep =   0
  Target State =   1 Target Symmetry =   2
  MOs for active space:   2  17     MOs for small active space:   2  17
  Spin state        Sol. of Reference-CI       Sol. of A-CI and B-CI     MaxR
  Singlet            0  1  0  0                 0  1  0  0               2
Singlet
  B-operator: SDCI for reference-CI with small active space
  Generate all the higher-order excitation operators
  Skip higher-order unlinked terms
***********************************************
              SINGLET STATE
***********************************************
STEP #MEGI# : Calculation of integrals for REFERENCE-CI ... DONE
STEP #DAS#  : Direct diagonalization for reference-CI ... Done
=====================================================================
  STEP #GHPRES#  Generation of A-CI, B-CI operators and selection
=====================================================================
*Reference configurations for Singlet       A2
    1:   3   5   3   4                2:   3   7   3   5
    3:   3   8   3   4                4:   3   5   2   4
    5:   3   4   2   5
  Square norm of reference state with above configurations:
   1: 0.97806
-------------------------------------------------------------
LINKED OPERATORS FOR SAC-CI: SYMMETRY = A2  EXCITED STATE
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE             2          96           98
    AFTER              2          64           66
STEP #MEGI# : Calculation of integrals for SDCI ... DONE
Solution for Singlet   A2    CONVERGED
STEP #SCIV# :   Iterative diagonalization for SD-CI ... Done
=================================================================
  STEP #EGOP#  Exponential generation of higher-operators
=================================================================
All the higher-order excitation operators are generated.
Perturbation selection with reference states
 Threshold for perturbation selection, EThreEgR (Lambda_E)   0.10D-05(AU)
== Estimation of full dimensions ==
 3-Ples:      3264   4-Ples:      6936
-------------------------------------------------------------------------
=================================================================
  STEP #MEGI#  Calculates CI matrix elements
=================================================================
```

Number of the linked operators for single- and double- excitation operators in SAC-CI w.f. before and after the perturbation selection

```
=============================================================
  STEP #MEGI#  Calculates unlinked integrals
=============================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
=============================================================
  STEP #SCIV#  Iterative diagonalization OF SAC-CI-V
=============================================================
Threshold for density convergence (DConvDiag) .10
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A2    CONVERGED
**********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
**********************************************
**********************************************
Singlet        A2      ************************
###   1-st  ###           ---   1st state in this spin                  y ---
    This state is being used for optimizations.
    Total energy       in au =     -24.955769
    Correlation energy in au =       0.167567
    Excitation energy  in au =       0.24913      in eV =       6.779170
  *SINGLE EXCITATION
       3   15       -0.04676
  *DOUBLE EXCITATION
       3    5    3    4   0.89764         3    8    3    4   0.28790
       3    7    3    5   0.28790         3    5    2    4  -0.10491
       3    4    2    5  -0.10491         2    5    2    4  -0.07858
       3    4    2    8  -0.04095         3    5    2    7  -0.04095
       3   12    2    5   0.03542         3   13    2    4   0.03542
=============================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
=============================================================
Energy gradient for SINGLET STATE        A2   1-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-CI-GR-V)=    0.1675673368 Total energy=       -24.9557694667
Z-vector iteration Converged
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-CI-V / SAC-NV density.
Gamma from SAC-CI General-R- V(singlet). Symmetry  2
With HF: IHF=         1 NDTEX=        66
Start back-transformation.
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     231
Number of TU pair in the last loop  =     231
```

SAC-CI result. This state is the target state of the geometry oprimization. Total energy, correlation energy (HF energy as the reference), excitation energy (SAC total energy as the reference), and the SAC-CI coefficients are shown. The 1^1A_1 state is characterized as two-electron excitation from 3-rd MO to 5- and 4-th MOs, and its coefficients is 0.89. The excitation energy is 6.78 eV.

```
Second-half back-transformation finished.
Use canonical orbitals for SAC/SAC-CI optimization.
Tollerance for orbital energy difference is  0.100D-08
Warning: This can cause divergence of gradients.
Max orbital gradient: YijMax=  0.000425 YabMax=  0.001046
DoAtom=TT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      847150.
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
Inv2:  IOpt= 1 Iter= 1 AM= 2.65D-16 Conv= 1.00D-12.
Inverted reduced A of dimension    8 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.

**********************************************************************

           Population analysis using the SCF density.

**********************************************************************

Orbital symmetries:
      Occupied  (SG) (SG) (SG)
      Virtual   (PI) (PI) (SG) (PI) (PI) (SG) (SG) (SG) (PI) (PI)
                (DLTA) (DLTA) (SG) (PI) (PI) (SG) (SG) (SG)
The electronic state is 1-SG.
Alpha  occ. eigenvalues --   -7.68806  -0.65982  -0.34280
Alpha virt. eigenvalues --    0.04885   0.04885   0.22465   0.35251   0.35251
Alpha virt. eigenvalues --    0.41580   0.47365   1.24530   1.59015   1.59015
Alpha virt. eigenvalues --    1.74820   1.74820   2.06748   2.45977   2.45977
Alpha virt. eigenvalues --    3.30089   4.76964  20.46702
         Condensed to atoms (all electrons):
             1          2
    1  B    4.671320   0.299095
    2  H    0.299095   0.730491
Mulliken atomic charges:
             1
    1  B    0.029585
    2  H   -0.029585
Sum of Mulliken charges=   0.00000
```

```
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  B    0.000000
    2  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    21.8244
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     0.0000    Y=     0.0000    Z=    -2.0878  Tot=     2.0878
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -6.5054   YY=    -6.5054   ZZ=   -10.6155
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=     1.3700   YY=     1.3700   ZZ=    -2.7401
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=     0.0000  YYY=     0.0000  ZZZ=    -6.5665  XYY=     0.0000
 XXY=     0.0000  XXZ=    -1.6113  XZZ=     0.0000  YZZ=     0.0000
 YYZ=    -1.6113  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=    -8.6284 YYYY=    -8.6284 ZZZZ=   -27.2484 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=    -2.8761 XXZZ=    -5.9830 YYZZ=    -5.9830
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 2.211724518515D+00 E-N=-6.242547858997D+01  KE= 2.513671486323D+01
Symmetry A1   KE= 2.513671486323D+01
Symmetry A2   KE= 0.000000000000D+00
Symmetry B1   KE= 0.000000000000D+00
Symmetry B2   KE= 0.000000000000D+00
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          5           0.000000000    0.000000000    0.002894768
   2          1           0.000000000    0.000000000   -0.002894768
-------------------------------------------------------------------
Cartesian Forces:  Max     0.002894768 RMS     0.001671295

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.002894768 RMS     0.002894768
Search for a local minimum.
Step number   1 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- first step.
The second derivative matrix:
                          R1
          R1           0.24937
```

Energy gradient in cartesian coordinate calculated at the initial geometry.

```
    Eigenvalues ---    0.24937
RFO step:  Lambda=-3.35984262D-05.
Linear search not attempted -- first point.
Iteration  1 RMS(Cart)=  0.00820711 RMS(Int)=  0.00000000
Iteration  2 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.26068  -0.00289   0.00000  -0.01161  -0.01161   2.24907
        Item               Value     Threshold  Converged?
Maximum Force            0.002895     0.000450     NO
RMS     Force            0.002895     0.000300     NO
Maximum Displacement     0.005803     0.001800     NO
RMS     Displacement     0.008207     0.001200     NO
Predicted change in Energy=-1.680148D-05
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5            0        0.000000    0.000000    0.003071
   2          1            0        0.000000    0.000000    1.193229
---------------------------------------------------------------------
Stoichiometry    BH
Framework group  C*V[C*(HB)]
Deg. of freedom     1
Full point group                 C*V     NOp   4
Largest Abelian subgroup         C2V     NOp   4
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5            0        0.000000    0.000000    0.198360
   2          1            0        0.000000    0.000000   -0.991798
---------------------------------------------------------------------
Rotational constants (GHZ):      0.0000000    386.4235915    386.4235915
Standard basis: D95(d,p) (6D, 7F)
There are    12 symmetry adapted basis functions of A1  symmetry.
There are     1 symmetry adapted basis functions of A2  symmetry.
There are     4 symmetry adapted basis functions of B1  symmetry.
There are     4 symmetry adapted basis functions of B2  symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   21 basis functions,    37 primitive gaussians,    21 cartesian basis functions
    3 alpha electrons        3 beta electrons
```

Energy gradient and displacements do not satisfy convergence criteria.

The second geometry to be calculated.

```
      nuclear repulsion energy         2.2231383817 Hartrees.
NAtoms=    2 NActive=    2 NUniq=    2 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    21 RedAO= T  NBF=    12     1     4     4
NBsUse=    21 1.00D-06 NBFU=    12     1     4     4
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (SG) (SG) (SG)
      Virtual   (PI) (PI) (SG) (PI) (PI) (SG) (SG) (SG) (PI) (PI)
                (DLTA) (DLTA) (SG) (PI) (PI) (SG) (SG) (SG)
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=      871060.
SCF Done:  E(RHF) =  -25.1231312155     A.U. after    7 cycles
            Convg  =    0.1836D-08             -V/T =  1.9992
            S**2   =   0.0000
Perform MO ordering.
Number of Electrons          6
Spin Multiplicity            1
Number of Occupieds          3
Number of Molecular Charge   0
Use orbital energies in MO ordering; INotEig=    0.
Use dipole moments in MO ordering; IFlagDP=    1.
Use second moments in MO ordering; IFlagSM=    1.
ExpMin= 7.01D-02 ExpMax= 2.79D+03 ExpMxC= 4.19D+02 IAcc=3 IRadAn=         5 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=         5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     2    20
NBasis=    21 NAE=     3 NBE=     3 NFC=     1 NFV=     1
NROrb=     19 NOA=     2 NOB=     2 NVA=    17 NVB=    17
No. of INTEGRALS =      5257 NBLK =         3 KOUNT =       457
  Calculate the SAC-CI general-R gradients. IGROpt=   1
*****************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 1
*****************************************************************************
==============================================================
  STEP #PRES#  Generation of Linked Operators and Selection
==============================================================
== States to be calculated ==
           A1   A2   B1   B2
SINGLET    Yes  No   No   No
TRIPLET    No   No   No   No
IONIZED    No   No   No   No
ANIONIZED  No   No   No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,   0,   0,   0)
```

```
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
  ---------------------------------------------------------------
   During geometry optimization, the same linked and unlinked
   operators are used.
  ---------------------------------------------------------------
****************************
        SINGLET STATE
****************************
================================================================
  STEP #CIMX#  CI matrix elements         ### SINGLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A1    CONVERGED
================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
================================================================
================================================================
  STEP #SAC#  Solution of SAC equation
================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*********************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*********************************************
HF ENERGY     =     -25.123131 (AU)
SAC-NV  ENERGY=      -0.081520 (AU)
TOTAL ENERGY  =     -25.204651 (AU)
*******************************************************************************
    SAC-CI GENERAL-R  Geometry optimization. IStep= 1
*******************************************************************************
SINGLET STATE
  Number of States  Singlet       =(  0  1  0  0)
  Perturbation selection with reference state
   Threshold of perturbation selection of linked operator # LevelThree #
    EThreR2(E) (Lambda_E)=  0.100D-06(au)
   Spin functions of selected operators may be incomplete.
  Calculate SAC-CI general-R gradients. IStep =   1
  Target State =   1 Target Symmetry =   2
```

```
  MOs for active space:   2  17     MOs for small active space:   2  17
  Spin state        Sol. of Reference-CI       Sol. of A-CI and B-CI     MaxR
  Singlet            0  1  0  0                 0  1  0  0               2
Singlet
  B-operator: SDCI for reference-CI with small active space
  Generate all the higher-order excitation operators
  Skip higher-order unlinked terms
STEP #MEGI# : Calculation of integrals for REFERENCE-CI ... DONE
STEP #DAS#  : Direct diagonalization for reference-CI ... Done
=====================================================================
  STEP #GHPRES#  Generation of A-CI, B-CI operators and selection
=====================================================================
STEP #MEGI# : Calculation of integrals for SDCI ... DONE
Solution for Singlet   A2    CONVERGED
STEP #SCIV# :   Iterative diagonalization for SD-CI ... Done
=============================================================
  STEP #MEGI#  Calculates CI matrix elements
=============================================================
=============================================================
  STEP #MEGI#  Calculates unlinked integrals
=============================================================
Thresholds for R1,R2 operators (CThreULR1,CThreULR2) 0.500D-01 0.500D-01
Threshold for S2 operators (CThreULS2) 0.000D+00
=============================================================
  STEP #SCIV#  Iterative diagonalization OF SAC-CI-V
=============================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A2    CONVERGED
**********************************************
   ENERGY AND WAVE FUNCTION OF SAC-CI METHOD
**********************************************
*****************************************************************************
Singlet        A2      ***********************************************************
###   1-st  ###          ---   1st state in this spin multiplicity ---
    This state is being used for optimizations.
    Total energy       in au =     -24.955785
    Correlation energy in au =       0.167346
    Excitation energy  in au =       0.248866    in eV =       6.771983
  *SINGLE EXCITATION
       3   15       -0.04675
  *DOUBLE EXCITATION
       3    5    3    4   0.89716         3    8    3    4   0.28841
       3    7    3    5   0.28841         3    4    2    5  -0.10651
       3    5    2    4  -0.10651         2    5    2    4  -0.07770
       3    5    2    7  -0.04180         3    4    2    8  -0.04180
       3   13    2    4   0.03540         3   12    2    5   0.03540
=============================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
```

SAC-CI result at the updated geometry. The total energy is decreasing compared with that at the last geometry (-24.955769 au). The excitation energy calculated with the SD-R method is higher than that with general-R method by 0.6 eV. Since the target state is two-electron process, including triples significantly improves the excitation energy.

```
=================================================================
Energy gradient for SINGLET STATE        A2   1-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-CI-GR-V)=    0.1673461317 Total energy=       -24.9557850837
Z-vector iteration Converged
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-CI-V / SAC-NV density.
Gamma from SAC-CI General-R- V(singlet). Symmetry  2
With HF: IHF=         1 NDTEX=        66
Start back-transformation.
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     231
Number of TU pair in the last loop  =     231
Second-half back-transformation finished.
Use canonical orbitals for SAC/SAC-CI optimization.
Tollerance for orbital energy difference is  0.100D-08
Warning: This can cause divergence of gradients.
Max orbital gradient: YijMax=  0.000421 YabMax=  0.001053
DoAtom=TT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      847150.
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
Inv2:  IOpt= 1 Iter= 1 AM= 3.84D-16 Conv= 1.00D-12.
Inverted reduced A of dimension    8 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          5           0.000000000    0.000000000   -0.000221622
   2          1           0.000000000    0.000000000    0.000221622
-------------------------------------------------------------------
```

Energy gradient in cartesian coordinate calculated at the updated geometry.

```
Cartesian Forces:  Max     0.000221622 RMS     0.000127953

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Berny optimization.
Internal  Forces:  Max     0.000221622 RMS     0.000221622
Search for a local minimum.
Step number   2 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using D2CorX and points  1  2
Trust test= 9.30D-01 RLast= 1.16D-02 DXMaxT set to 3.00D-01
The second derivative matrix:
                          R1
          R1           0.26850
    Eigenvalues ---    0.26850
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.06999.
Iteration  1 RMS(Cart)=  0.00057441 RMS(Int)=  0.00000000
Iteration  2 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.24907   0.00022   0.00081   0.00000   0.00081   2.24989
        Item               Value     Threshold  Converged?
Maximum Force            0.000222     0.000450     YES
RMS     Force            0.000222     0.000300     YES
Maximum Displacement     0.000406     0.001800     YES
RMS     Displacement     0.000574     0.001200     YES
Predicted change in Energy=-9.144052D-08
Optimization completed.
   -- Stationary point found.
                          ----------------------------
                          !   Optimized Parameters   !
                          ! (Angstroms and Degrees)  !
--------------------------                            --------------------
! Name  Definition              Value          Derivative Info.
--------------------------------------------------------------------------
! R1    R(1,2)                  1.1902         -DE/DX =    0.0002
!------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic             Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5          0        0.000000    0.000000    0.003071
   2          1          0        0.000000    0.000000    1.193229
---------------------------------------------------------------------
Stoichiometry    BH
Framework group  C*V[C*(HB)]
```

Energy gradient and displacements satisfy convergence criteria.

Optimized B-H bond distance. This reasonably reproduces the experimental value (1.196 ang.). General-R result in the last example shows better agreement (1.199 ang.)

```
Deg. of freedom     1
Full point group                 C*V     NOp   4
Largest Abelian subgroup         C2V     NOp   4
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5            0        0.000000    0.000000    0.198360
   2          1            0        0.000000    0.000000   -0.991798
---------------------------------------------------------------------
Rotational constants (GHZ):      0.0000000    386.4235915    386.4235915

*********************************************************************

           Population analysis using the SCF density.

*********************************************************************

Orbital symmetries:
      Occupied  (SG) (SG) (SG)
      Virtual   (PI) (PI) (SG) (PI) (PI) (SG) (SG) (SG) (PI) (PI)
                (DLTA) (DLTA) (SG) (PI) (PI) (SG) (SG) (SG)
The electronic state is 1-SG.
Alpha  occ. eigenvalues --   -7.68738  -0.66148  -0.34259
Alpha virt. eigenvalues --    0.04895   0.04895   0.22414   0.35266   0.35266
Alpha virt. eigenvalues --    0.41866   0.47379   1.24576   1.58958   1.58958
Alpha virt. eigenvalues --    1.74847   1.74847   2.07560   2.46520   2.46520
Alpha virt. eigenvalues --    3.31151   4.76984  20.46742
         Condensed to atoms (all electrons):
             1          2
    1  B    4.673207   0.299536
    2  H    0.299536   0.727721
Mulliken atomic charges:
             1
    1  B    0.027257
    2  H   -0.027257
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  B    0.000000
    2  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    21.7629
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     0.0000    Y=     0.0000    Z=    -2.1064  Tot=     2.1064
Quadrupole moment (field-independent basis, Debye-Ang):
```

```
  XX=    -6.4995   YY=    -6.4995   ZZ=   -10.6031
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=     1.3678   YY=     1.3678   ZZ=    -2.7357
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=     0.0000  YYY=     0.0000  ZZZ=    -6.6008  XYY=     0.0000
 XXY=     0.0000  XXZ=    -1.6243  XZZ=     0.0000  YZZ=     0.0000
 YYZ=    -1.6243  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=    -8.6219 YYYY=    -8.6219 ZZZZ=   -27.1135 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=    -2.8740 XXZZ=    -5.9598 YYZZ=    -5.9598
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 2.223138381670D+00 E-N=-6.245215896465D+01  KE= 2.514250244891D+01
Symmetry A1   KE= 2.514250244891D+01
Symmetry A2   KE= 4.815442214459D-51
Symmetry B1   KE= 0.000000000000D+00
Symmetry B2   KE= 0.000000000000D+00
Final structure in terms of initial Z-matrix:
B
H,1,BH
     Variables:
BH=1.19015805

Test job not archived.
1¥1¥GINC-MIRAI86¥FOpt¥RSACCI¥D95(d,p)¥B1H1¥MASAHIRO¥03-Aug-2004¥0¥¥# S
AC-CI(SINGLET=(NSTATE=(0,1,0,0),MAXR=2), TARGETSTATE=(SPINSTATE=SINGLE
T,SYMMETRY=2,ROOT=1), GENERAL-R) /D95** OPT CPHF=CANONICAL TEST¥¥Gauss
ian Test Job 647 (Part 2): SAC-CI SD-R geometry optimization calculati
on for the singlet Delta excited state of BH with full-valence active
MOs of D95**. Initial geometry is the experimental one.¥¥0,1¥B,0.,0.,-
0.198359675¥H,0.,0.,0.9917983751¥¥Version=AI64T-G03RevC.02¥State=1-SG¥
HF=-25.1231312¥RMSD=1.836e-09¥RMSF=1.280e-04¥Dipole=0.,0.,-0.2702437¥P
G=C*V [C*(H1B1)]¥¥@


NOTHING RESEMBLES A NEW PHENOMENON AS MUCH AS A MISTAKE.

                                -- ENRICO FERMI (?)
Job cpu time:  0 days  0 hours  0 minutes 14.9 seconds.
File lengths (MBytes):  RWF=    114 Int=      0 D2E=      0 Chk=     10 Scr=     28
Normal termination of Gaussian 03 at Tue Aug  3 13:36:43 2004.
Initial command:
/work/g03.C02/g03/l1.exe /work/g03.C02/inputs/Gau-185105.inp -scrdir=/work/g03.C02/inputs/
Entering Link 1 = /work/g03.C02/g03/l1.exe PID=    185117.

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```

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```
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O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

****************************************
Gaussian 03:  AI64T-G03RevC.02 12-Jun-2004
                3-Aug-2004
****************************************
%mem=12mw
---------------------------------------------------------------------------
# SAC-CI(SacOnly, TargetState=(SpinState=Singlet,Symmetry=1,Root=0)) /
D95** Opt CPHF=Canonical test
---------------------------------------------------------------------------

Warning:  CPHF=MOD not CPHF=Canonical is strongly recommended with GSUM.
1/18=20,38=1/1,3;
2/9=110,17=6,18=5,40=1/2;
3/5=8,7=101,11=9,16=1,25=1,30=1,36=2/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=5,9=30000,10=1,40=1,42=1/1,4;
9/15=1/23;
11/28=-13,29=200,42=3,46=1/11;
10/5=5/2;
6/7=2,8=2,9=2,10=2/1;
7/12=7/1,2,3,16;
1/18=20/3(1);
99//99;
2/9=110/2;
3/5=8,7=101,11=9,16=1,25=1,30=1,36=2/1,2,3;
4/5=5,16=3/1;
5/5=2,38=5/2;
8/6=5,9=30000,10=1,40=1,42=1/1,4;
9/15=1/23;
```

List of keywords given in the Gaussian input. This example calculates the ground state geometry with the SD-R method. The result is also used for calculating adiabatic excitation energy.

```
11/28=-13,29=200,42=3,46=1/11;
10/5=5/2;
7/12=7/1,2,3,16;
1/18=20/3(-9);
2/9=110/2;
6/7=2,8=2,9=2,10=2/1;
99//99;
-----------------------------------------------------------------------
Gaussian Test Job 647 (Part 3): Geometry optimization calculation of t
he SAC ground state of BH with full-valence active MOs of D95**. Initi
al geometry is the experimental one.
-----------------------------------------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
B
H                    1    BH
      Variables:
 BH                    1.232


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Berny optimization.
Initialization pass.
                           ----------------------------
                           !    Initial Parameters    !
                           ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
-------------------------------------------------------------------------------
! R1    R(1,2)                  1.232          estimate D2E/DX2                !
-------------------------------------------------------------------------------
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5            0        0.000000    0.000000    0.000000
   2          1            0        0.000000    0.000000    1.232000
---------------------------------------------------------------------
Stoichiometry    BH
Framework group  C*V[C*(HB)]
Deg. of freedom     1
Full point group                 C*V     NOp   4
Largest Abelian subgroup         C2V     NOp   4
Largest concise Abelian subgroup C1      NOp   1
```

```
                    Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5            0        0.000000    0.000000    0.205333
   2          1            0        0.000000    0.000000   -1.026667
---------------------------------------------------------------------
Rotational constants (GHZ):      0.0000000    360.6213990    360.6213990
Standard basis: D95(d,p) (6D, 7F)
There are    12 symmetry adapted basis functions of A1  symmetry.
There are     1 symmetry adapted basis functions of A2  symmetry.
There are     4 symmetry adapted basis functions of B1  symmetry.
There are     4 symmetry adapted basis functions of B2  symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   21 basis functions,    37 primitive gaussians,    21 cartesian basis functions
    3 alpha electrons        3 beta electrons
      nuclear repulsion energy         2.1476347739 Hartrees.
NAtoms=    2 NActive=    2 NUniq=    2 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    21 RedAO= T  NBF=    12     1     4     4
NBsUse=    21 1.00D-06 NBFU=    12     1     4     4
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 7.01D-02 ExpMax= 2.79D+03 ExpMxC= 4.19D+02 IAcc=2 IRadAn=         4 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Initial guess orbital symmetries:
      Occupied  (SG) (SG) (SG)
      Virtual   (PI) (PI) (SG) (SG) (PI) (PI) (SG) (SG) (PI) (PI)
                (DLTA) (DLTA) (SG) (PI) (PI) (SG) (SG) (SG)
The electronic state of the initial guess is 1-SG.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=      871060.
SCF Done:  E(RHF) =  -25.1238792455     A.U. after    8 cycles
            Convg  =    0.7835D-08             -V/T =  2.0008
            S**2   =   0.0000
Perform MO ordering.
ExpMin= 7.01D-02 ExpMax= 2.79D+03 ExpMxC= 4.19D+02 IAcc=3 IRadAn=         5 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=         5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     2    20
NBasis=    21 NAE=     3 NBE=     3 NFC=     1 NFV=     1
NROrb=     19 NOA=     2 NOB=     2 NVA=    17 NVB=    17
---------------------------------------------------------------------
```

```
#####################################################################
---------------------------------------------------------------------
              SAC/SAC-CI Program Combined with GAUSSIAN
                            for Calculating
        Ground, Excited, Ionized, and Electron-Attached States
                                and
             Singlet, Doublet, Triplet, Quartet, Quintet,
                   Sextet, and Septet Spin States
                                and
                 Their Analytical Energy Gradients
                        coded originally by
                         Hiroshi Nakatsuji
                          and extended by
 H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa,
      M. Ishida, T. Nakajima, Y. Honda, O. Kitao, and H. Nakai
                                at
                 Department of Hydrocarbon Chemistry,
               Division of Molecular Engineering, and
      Department of Synthetic Chemistry & Biological Chemistry,
                 Graduate School of Engineering,
                        Kyoto University,
                      Kyoto 606-8501, Japan
---------------------------------------------------------------------
#####################################################################
---------------------------------------------------------------------
No. of INTEGRALS =      5257 NBLK =         3 KOUNT =       457
*****************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 0
*****************************************************************************
===============================================================
  STEP #PRES#  Generation of Linked Operators and Selection
===============================================================
 C*v    -> C2v     *=infinity
-------------------
 Sigma+ -> A1
 Sigma- -> A2
 Pi     -> B1 + B2
 Delta  -> A1 + A2
   ...
PERTURBATION SELECTION FOR THE DEGENERATE SYMMETRY
== States to be calculated ==
           A1   A2   B1   B2
SINGLET    Yes  No   No   No
TRIPLET    No   No   No   No
IONIZED    No   No   No   No
ANIONIZED  No   No   No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,   0,   0,   0)
```

```
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
****************************
        SINGLET STATE
****************************
------------------------------------------------------------
LINKED OPERATORS FOR SAC:    SYMMETRY = A1  GROUND STATE
  SELECTION        SINGLE      DOUBLE       TOTAL
    BEFORE            16         211          227
    AFTER             16         178          195
DEGENERACY IS CONSIDERED FOR SYMMETRY B1  B2
================================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A1    CONVERGED
================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
================================================================
Threshold for S2 operator (CThreULS2G) 0.500D-02
================================================================
  STEP #SAC#  Solution of SAC equation
================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*********************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*********************************************
HF ENERGY     =     -25.123879 (AU)
SAC-NV  ENERGY=      -0.081875 (AU)
TOTAL ENERGY  =     -25.205754 (AU)
SAC-NV  coefficients (|C|>=0.03)
*SINGLE EXCITATION
*DOUBLE EXCITATION
       3    5    3    5     -0.11053         3    4    3    4     -0.11053
       3    8    3    5     -0.10495         3    7    3    4     -0.10495
       3    5    2    5     -0.08591         3    4    2    4     -0.08591
       3    9    2    9      0.05962         3   10    3    9      0.05341
       2    8    2    5     -0.05331         2    7    2    4     -0.05331
```

Number of the linked operators for single- and double- excitation operators in the SAC w.f. before and after the perturbation selection

Result of SAC calculation. Hartree-Fock (HF) energy, SAC-NV energy (correlation energy obtained with the SAC method), and the SAC-NV coefficients are shown. HF configuration always has 1.00 in the SAC wave function.

```
       2    9    2    9     -0.05216         3    8    2    5     -0.05180
       3    7    2    4     -0.05180         3   10    3   10     -0.05104
       3    5    2    8     -0.05093         3    4    2    7     -0.05093
       3    9    3    9     -0.04453         3   13    3    5     -0.04427
       3   12    3    4     -0.04427         2    5    2    5     -0.04183
       2    4    2    4     -0.04183         2   16    2    9     -0.03269
       3    8    2    8     -0.03266         3    7    2    7     -0.03266
       3   11    2   11      0.03070         3   13    2    5     -0.03067
       3   12    2    4     -0.03067         3   10    3    6     -0.03010
       3   10    2   10     -0.03009
Hartree-Fock configuration   1.00000
=================================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
=================================================================
Energy gradient for SINGLET STATE A1   0-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-NV)=   -0.0818747233 Total energy=       -25.2057539688
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-NV density.
Start back-transformation.
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     231
Number of TU pair in the last loop  =     231
Second-half back-transformation finished.
Use canonical orbitals for SAC/SAC-CI optimization.
Tollerance for orbital energy difference is  0.100D-08
Warning: This can cause divergence of gradients.
Max orbital gradient: YijMax=  0.000017 YabMax=  0.000020
DoAtom=TT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      847150.
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
```

```
Inv2:  IOpt= 1 Iter= 1 AM= 2.92D-16 Conv= 1.00D-12.
Inverted reduced A of dimension    8 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.

*********************************************************************

          Population analysis using the SCF density.

*********************************************************************

Orbital symmetries:
      Occupied  (SG) (SG) (SG)
      Virtual   (PI) (PI) (SG) (PI) (PI) (SG) (SG) (SG) (PI) (PI)
                (DLTA) (DLTA) (SG) (PI) (PI) (SG) (SG) (SG)
The electronic state is 1-SG.
Alpha  occ. eigenvalues --   -7.69208  -0.65042  -0.34399
Alpha virt. eigenvalues --    0.04821   0.04821   0.22744   0.35161   0.35161
Alpha virt. eigenvalues --    0.39939   0.47303   1.24267   1.59428   1.59428
Alpha virt. eigenvalues --    1.74659   1.74659   2.02128   2.42904   2.42904
Alpha virt. eigenvalues --    3.23976   4.76748  20.46509
         Condensed to atoms (all electrons):
             1          2
    1  B    4.660842   0.296716
    2  H    0.296716   0.745726
Mulliken atomic charges:
             1
    1  B    0.042442
    2  H   -0.042442
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  B    0.000000
    2  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    22.1878
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     0.0000    Y=     0.0000    Z=    -1.9774  Tot=     1.9774
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -6.5397   YY=    -6.5397   ZZ=   -10.6887
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=     1.3830   YY=     1.3830   ZZ=    -2.7660
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=     0.0000  YYY=     0.0000  ZZZ=    -6.3589  XYY=     0.0000
 XXY=     0.0000  XXZ=    -1.5337  XZZ=     0.0000  YZZ=     0.0000
 YYZ=    -1.5337  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
```

```
XXXX=    -8.6681 YYYY=    -8.6681 ZZZZ=   -28.0544 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=    -2.8894 XXZZ=    -6.1215 YYZZ=    -6.1215
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 2.147634773945D+00 E-N=-6.227488917775D+01  KE= 2.510485711898D+01
Symmetry A1   KE= 2.510485711898D+01
Symmetry A2   KE=-4.815442214459D-51
Symmetry B1   KE= 0.000000000000D+00
Symmetry B2   KE= 0.000000000000D+00
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          5           0.000000000    0.000000000   -0.004656746
   2          1           0.000000000    0.000000000    0.004656746
-------------------------------------------------------------------
Cartesian Forces:  Max     0.004656746 RMS     0.002688574

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.004656746 RMS     0.004656746
Search for a local minimum.
Step number   1 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- first step.
The second derivative matrix:
                          R1
          R1           0.22470
    Eigenvalues ---    0.22470
RFO step:  Lambda=-9.64682641D-05.
Linear search not attempted -- first point.
Iteration  1 RMS(Cart)=  0.01464829 RMS(Int)=  0.00000000
Iteration  2 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.32814   0.00466   0.00000   0.02072   0.02072   2.34886
        Item               Value     Threshold  Converged?
Maximum Force            0.004657     0.000450     NO
RMS     Force            0.004657     0.000300     NO
Maximum Displacement     0.010358     0.001800     NO
RMS     Displacement     0.014648     0.001200     NO
Predicted change in Energy=-4.825483D-05
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
-------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
```

Energy gradient calculated at the initial geometry.

Energy gradient and displacements do not satisfy convergence criteria.

```
---------------------------------------------------------------------
   1          5             0        0.000000    0.000000   -0.005481
   2          1             0        0.000000    0.000000    1.237481
---------------------------------------------------------------------
Stoichiometry    BH
Framework group  C*V[C*(HB)]
Deg. of freedom     1
Full point group                 C*V     NOp   4
Largest Abelian subgroup         C2V     NOp   4
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5             0        0.000000    0.000000    0.207160
   2          1             0        0.000000    0.000000   -1.035802
---------------------------------------------------------------------
Rotational constants (GHZ):      0.0000000    354.2884327    354.2884327
Standard basis: D95(d,p) (6D, 7F)
There are    12 symmetry adapted basis functions of A1  symmetry.
There are     1 symmetry adapted basis functions of A2  symmetry.
There are     4 symmetry adapted basis functions of B1  symmetry.
There are     4 symmetry adapted basis functions of B2  symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   21 basis functions,    37 primitive gaussians,    21 cartesian basis functions
    3 alpha electrons        3 beta electrons
      nuclear repulsion energy         2.1286936613 Hartrees.
NAtoms=    2 NActive=    2 NUniq=    2 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    21 RedAO= T  NBF=    12     1     4     4
NBsUse=    21 1.00D-06 NBFU=    12     1     4     4
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (SG) (SG) (SG)
      Virtual   (PI) (PI) (SG) (PI) (PI) (SG) (SG) (SG) (PI) (PI)
                (DLTA) (DLTA) (SG) (PI) (PI) (SG) (SG) (SG)
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=      871060.
SCF Done:  E(RHF) =  -25.1238406368     A.U. after    7 cycles
            Convg  =    0.3309D-08             -V/T =  2.0011
            S**2   =   0.0000
Perform MO ordering.
Number of Electrons          6
```

The second geometry to be calculated.

```
Spin Multiplicity            1
Number of Occupieds          3
Number of Molecular Charge   0
Use orbital energies in MO ordering; INotEig=    0.
Use dipole moments in MO ordering; IFlagDP=    1.
Use second moments in MO ordering; IFlagSM=    1.
ExpMin= 7.01D-02 ExpMax= 2.79D+03 ExpMxC= 4.19D+02 IAcc=3 IRadAn=        5 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=        5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     2    20
NBasis=    21 NAE=     3 NBE=     3 NFC=     1 NFV=     1
NROrb=     19 NOA=     2 NOB=     2 NVA=    17 NVB=    17
No. of INTEGRALS =      5257 NBLK =         3 KOUNT =       457
*******************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 1
*******************************************************************************
================================================================
  STEP #PRES#  Generation of Linked Operators and Selection
================================================================
== States to be calculated ==
           A1   A2   B1   B2
SINGLET    Yes  No   No   No
TRIPLET    No   No   No   No
IONIZED    No   No   No   No
ANIONIZED  No   No   No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  0,  0,  0)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
  ---------------------------------------------------------------
   During geometry optimization, the same linked and unlinked
   operators are used.
  ---------------------------------------------------------------
*****************************
        SINGLET STATE
*****************************
================================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A1    CONVERGED
================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
```

```
=================================================================
=================================================================
  STEP #SAC#  Solution of SAC equation
=================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*******************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*******************************************
HF ENERGY     =     -25.123841 (AU)
SAC-NV  ENERGY=      -0.081966 (AU)
TOTAL ENERGY  =     -25.205807 (AU)
SAC-NV  coefficients (|C|>=0.03)
*SINGLE EXCITATION
*DOUBLE EXCITATION
       3    4    3    4     -0.10978         3    5    3    5     -0.10978
       3    7    3    4     -0.10423         3    8    3    5     -0.10423
       3    4    2    4     -0.08683         3    5    2    5     -0.08683
       3    9    2    9      0.06101         3   10    3    9      0.05449
       2    8    2    5     -0.05374         2    7    2    4     -0.05374
       2    9    2    9     -0.05258         3    7    2    4     -0.05240
       3    8    2    5     -0.05240         3    4    2    7     -0.05141
       3    5    2    8     -0.05141         3   10    3   10     -0.05005
       3    9    3    9     -0.04635         3   12    3    4     -0.04400
       3   13    3    5     -0.04400         2    5    2    5     -0.04236
       2    4    2    4     -0.04236         3    7    2    7     -0.03292
       3    8    2    8     -0.03292         2   16    2    9     -0.03269
       3   11    2   11      0.03085         3   13    2    5     -0.03078
       3   12    2    4     -0.03078         3   10    2   10     -0.03055
Hartree-Fock configuration   1.00000
=================================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
=================================================================
Energy gradient for SINGLET STATE A1   0-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-NV)=   -0.0819663223 Total energy=       -25.2058069591
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-NV density.
Start back-transformation.
```

SAC result at the updated geometry. The total energy is decreasing compared with that at the last geometry (-25.205754 au).

```
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     231
Number of TU pair in the last loop  =     231
Second-half back-transformation finished.
Use canonical orbitals for SAC/SAC-CI optimization.
Tollerance for orbital energy difference is  0.100D-08
Warning: This can cause divergence of gradients.
Max orbital gradient: YijMax=  0.000019 YabMax=  0.000023
DoAtom=TT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      847150.
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
Inv2:  IOpt= 1 Iter= 1 AM= 1.65D-16 Conv= 1.00D-12.
Inverted reduced A of dimension    8 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
   1          5           0.000000000    0.000000000   -0.000498088
   2          1           0.000000000    0.000000000    0.000498088
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000498088 RMS     0.000287571

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.000498088 RMS     0.000498088
Search for a local minimum.
Step number   2 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using D2CorX and points  1  2
Trust test= 1.10D+00 RLast= 2.07D-02 DXMaxT set to 3.00D-01
The second derivative matrix:
                          R1
          R1           0.20075
    Eigenvalues ---    0.20075
```

Energy gradient in cartesian coordinate calculated at the updated geometry.

```
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of  0.12365.
Iteration  1 RMS(Cart)=  0.00181123 RMS(Int)=  0.00000000
Iteration  2 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.34886   0.00050   0.00256   0.00000   0.00256   2.35142
         Item               Value     Threshold  Converged?
Maximum Force            0.000498     0.000450     NO
RMS     Force            0.000498     0.000300     NO
Maximum Displacement     0.001281     0.001800     YES
RMS     Displacement     0.001811     0.001200     NO
Predicted change in Energy=-6.172711D-07
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5            0        0.000000    0.000000   -0.006159
   2          1            0        0.000000    0.000000    1.238159
---------------------------------------------------------------------
Stoichiometry    BH
Framework group  C*V[C*(HB)]
Deg. of freedom     1
Full point group                 C*V     NOp   4
Largest Abelian subgroup         C2V     NOp   4
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5            0        0.000000    0.000000    0.207386
   2          1            0        0.000000    0.000000   -1.036932
---------------------------------------------------------------------
Rotational constants (GHZ):      0.0000000    353.5169799    353.5169799
Standard basis: D95(d,p) (6D, 7F)
There are    12 symmetry adapted basis functions of A1  symmetry.
There are     1 symmetry adapted basis functions of A2  symmetry.
There are     4 symmetry adapted basis functions of B1  symmetry.
There are     4 symmetry adapted basis functions of B2  symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   21 basis functions,    37 primitive gaussians,    21 cartesian basis functions
    3 alpha electrons        3 beta electrons
      nuclear repulsion energy         2.1263748140 Hartrees.
```

Energy gradient and displacements do not satisfy convergence criteria.

The updated geometry to be calculated.

```
NAtoms=    2 NActive=    2 NUniq=    2 SFac= 1.00D+00 NAtFMM=   60 Big=F
One-electron integrals computed using PRISM.
NBasis=    21 RedAO= T  NBF=    12     1     4     4
NBsUse=    21 1.00D-06 NBFU=    12     1     4     4
Initial guess read from the read-write file:
Initial guess orbital symmetries:
      Occupied  (SG) (SG) (SG)
      Virtual   (PI) (PI) (SG) (PI) (PI) (SG) (SG) (SG) (PI) (PI)
                (DLTA) (DLTA) (SG) (PI) (PI) (SG) (SG) (SG)
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 integrals in memory in canonical form, NReq=      871060.
SCF Done:  E(RHF) =  -25.1238296759     A.U. after    6 cycles
            Convg  =    0.8923D-08             -V/T =  2.0012
            S**2   =   0.0000
Perform MO ordering.
Number of Electrons          6
Spin Multiplicity            1
Number of Occupieds          3
Number of Molecular Charge   0
Use orbital energies in MO ordering; INotEig=    0.
Use dipole moments in MO ordering; IFlagDP=    1.
Use second moments in MO ordering; IFlagSM=    1.
ExpMin= 7.01D-02 ExpMax= 2.79D+03 ExpMxC= 4.19D+02 IAcc=3 IRadAn=         5 AccDes= 0.00D+00
HarFok:  IExCor= 205 AccDes= 0.00D+00 IRadAn=         5 IDoV=1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Range of M.O.s used for correlation:     2    20
NBasis=    21 NAE=     3 NBE=     3 NFC=     1 NFV=     1
NROrb=     19 NOA=     2 NOB=     2 NVA=    17 NVB=    17
No. of INTEGRALS =      5257 NBLK =         3 KOUNT =       457
*****************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R)  Geometry optimization. IStep= 2
*****************************************************************************
===============================================================
  STEP #PRES#  Generation of Linked Operators and Selection
===============================================================
== States to be calculated ==
           A1   A2   B1   B2
SINGLET    Yes  No   No   No
TRIPLET    No   No   No   No
IONIZED    No   No   No   No
ANIONIZED  No   No   No   No
== Input data for perturbation selection ==
SINGLET STATE
 Number of States  Singlet      =(  1,  0,  0,  0)
 Perturbation selection for reference states.
 Threshold for perturbation selection of linked operator # LevelThree #
```

```
  EThreS2 (Lambda_G)=  0.100D-05(au)   EThreR2 (Lambda_E)=  0.100D-06(au)
  ---------------------------------------------------------------
   During geometry optimization, the same linked and unlinked
   operators are used.
  ---------------------------------------------------------------
****************************
        SINGLET STATE
****************************
================================================================
  STEP #CIMX#  CI matrix elements          ### SINGLET STATE ###
================================================================
================================================================
  STEP #DIAGCI#  Solution of SDCI
================================================================
Threshold for density convergence (DConvDiag) .100D-04
Maximum number of iteration (MaxItDiag)    64
Solution for Singlet   A1    CONVERGED
================================================================
  STEP #ULINTG#  Unlinked integral for Ground State (SAC)
================================================================
================================================================
  STEP #SAC#  Solution of SAC equation
================================================================
Threshold for norm convergence in SAC eq. (DConvSAC) .100D-06
Threshold for norm convergence in linear eq. (ConvLin) .100D-06
Maximum number of iteration in SAC eq. (MaxItSAC)    20
Maximum number of iteration in linear eq. (MaxItLin)   200
DIIS method is used.
Step #SAC# after #GSUM#
Solution for SAC equation converged
*********************************************
   ENERGY AND WAVE FUNCTION OF SAC METHOD
*********************************************
HF ENERGY     =     -25.123830 (AU)
SAC-NV  ENERGY=      -0.081978 (AU)
TOTAL ENERGY  =     -25.205808 (AU)
SAC-NV  coefficients (|C|>=0.03)
*SINGLE EXCITATION
*DOUBLE EXCITATION
       3    4    3    4     -0.10969         3    5    3    5     -0.10969
       3    7    3    4     -0.10414         3    8    3    5     -0.10414
       3    4    2    4     -0.08694         3    5    2    5     -0.08694
       3    9    2    9      0.06118         3   10    3    9      0.05462
       2    7    2    4     -0.05379         2    8    2    5     -0.05379
       2    9    2    9     -0.05264         3    7    2    4     -0.05247
       3    8    2    5     -0.05247         3    4    2    7     -0.05147
       3    5    2    8     -0.05147         3   10    3   10     -0.04993
       3    9    3    9     -0.04657         3   12    3    4     -0.04396
       3   13    3    5     -0.04396         2    4    2    4     -0.04243
```

SAC result at the updated geometry. The total energy is decreasing compared with that at the last geometry (-25.205807 au).

```
       2    5    2    5     -0.04243         3    8    2    8     -0.03295
       3    7    2    7     -0.03295         2   16    2    9     -0.03268
       3   11    2   11      0.03086         3   12    2    4     -0.03079
       3   13    2    5     -0.03079         3   10    2   10     -0.03060
Hartree-Fock configuration   1.00000
================================================================
  STEP #ZVECIT# Iterative Solution of CPSAC Z-Equation
================================================================
Energy gradient for SINGLET STATE A1   0-th solution
Threshold for norm convergence in macro iteration(EPSL) .100D-06
Threshold for norm convergence in micro iteration(EPSLZ).100D-06
Maximum number of iteration in macro iteration(MAXITL)   200
Maximum number of iteration in micro iteration(MAXITZ)  200
ECorr(SAC-NV)=   -0.0819779205 Total energy=       -25.2058075964
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
    0 densities were copied.
Do SAC-NV density.
Start back-transformation.
First-half back-transformation finished.
Number of loop for TU pair          =       1
Number of TU pair treated at a time =     231
Number of TU pair in the last loop  =     231
Second-half back-transformation finished.
Use canonical orbitals for SAC/SAC-CI optimization.
Tollerance for orbital energy difference is  0.100D-08
Warning: This can cause divergence of gradients.
Max orbital gradient: YijMax=  0.000019 YabMax=  0.000023
DoAtom=TT
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
         Store integrals in memory, NReq=      847150.
         There are   1 degrees of freedom in the 1st order CPHF.
    1 vectors were produced by pass  0.
AX will form   1 AO Fock derivatives at one time.
    1 vectors were produced by pass  1.
    1 vectors were produced by pass  2.
    1 vectors were produced by pass  3.
    1 vectors were produced by pass  4.
    1 vectors were produced by pass  5.
    1 vectors were produced by pass  6.
    1 vectors were produced by pass  7.
Inv2:  IOpt= 1 Iter= 1 AM= 3.04D-16 Conv= 1.00D-12.
Inverted reduced A of dimension    8 with in-core refinement.
End of Minotr Frequency-dependent properties file   721 does not exist.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                    Forces (Hartrees/Bohr)
```

Energy gradient in cartesian coordinate calculated at the updated geometry.

```
Number     Number              X              Y              Z
---------------------------------------------------------------------
   1          5           0.000000000    0.000000000    0.000000076
   2          1           0.000000000    0.000000000   -0.000000076
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000000076 RMS     0.000000044

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.000000076 RMS     0.000000076
Search for a local minimum.
Step number   3 out of a maximum of  20
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using D2CorX and points  2  3
Trust test= 1.03D+00 RLast= 2.56D-03 DXMaxT set to 3.00D-01
The second derivative matrix:
                          R1
          R1           0.19448
    Eigenvalues ---    0.19448
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.00015.
Iteration  1 RMS(Cart)=  0.00000028 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.35142   0.00000   0.00000   0.00000   0.00000   2.35142
        Item               Value     Threshold  Converged?
Maximum Force            0.000000     0.000450     YES
RMS     Force            0.000000     0.000300     YES
Maximum Displacement     0.000000     0.001800     YES
RMS     Displacement     0.000000     0.001200     YES
Predicted change in Energy=-1.481697D-14
Optimization completed.
   -- Stationary point found.
                          ----------------------------
                          !   Optimized Parameters   !
                          ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.2443         -DE/DX =    0.0                 !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5           0         0.000000    0.000000   -0.006159
```

Energy gradient and displacements satisfy convergence criteria.

Optimized B-H bond distance for the ground state.

```
   2          1             0        0.000000    0.000000    1.238159
---------------------------------------------------------------------
Stoichiometry    BH
Framework group  C*V[C*(HB)]
Deg. of freedom     1
Full point group                 C*V     NOp   4
Largest Abelian subgroup         C2V     NOp   4
Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          5             0        0.000000    0.000000    0.207386
   2          1             0        0.000000    0.000000   -1.036932
---------------------------------------------------------------------
Rotational constants (GHZ):      0.0000000    353.5169799    353.5169799

*********************************************************************

           Population analysis using the SCF density.

*********************************************************************

Orbital symmetries:
      Occupied  (SG) (SG) (SG)
      Virtual   (PI) (PI) (SG) (PI) (PI) (SG) (SG) (SG) (PI) (PI)
                (DLTA) (DLTA) (SG) (PI) (PI) (SG) (SG) (SG)
The electronic state is 1-SG.
Alpha  occ. eigenvalues --   -7.69348  -0.64727  -0.34439
Alpha virt. eigenvalues --    0.04798   0.04798   0.22833   0.35128   0.35128
Alpha virt. eigenvalues --    0.39387   0.47285   1.24180   1.59602   1.59602
Alpha virt. eigenvalues --    1.74601   1.74601   2.00576   2.41877   2.41877
Alpha virt. eigenvalues --    3.21897   4.76637  20.46458
         Condensed to atoms (all electrons):
             1          2
    1  B    4.657425   0.295967
    2  H    0.295967   0.750641
Mulliken atomic charges:
             1
    1  B    0.046608
    2  H   -0.046608
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  B    0.000000
    2  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=    22.3154
```

```
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     0.0000    Y=     0.0000    Z=    -1.9384  Tot=     1.9384
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -6.5516   YY=    -6.5516   ZZ=   -10.7143
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=     1.3876   YY=     1.3876   ZZ=    -2.7751
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=     0.0000  YYY=     0.0000  ZZZ=    -6.2840  XYY=     0.0000
 XXY=     0.0000  XXZ=    -1.5060  XZZ=     0.0000  YZZ=     0.0000
 YYZ=    -1.5060  XYZ=     0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=    -8.6825 YYYY=    -8.6825 ZZZZ=   -28.3413 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=    -2.8942 XXZZ=    -6.1708 YYZZ=    -6.1708
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 2.126374814048D+00 E-N=-6.222464937721D+01  KE= 2.509454011377D+01
Symmetry A1   KE= 2.509454011377D+01
Symmetry A2   KE= 0.000000000000D+00
Symmetry B1   KE= 0.000000000000D+00
Symmetry B2   KE= 0.000000000000D+00
Final structure in terms of initial Z-matrix:
B
H,1,BH
     Variables:
BH=1.24431781

Test job not archived.
1¥1¥GINC-MIRAI86¥FOpt¥RSACCI¥D95(d,p)¥B1H1¥MASAHIRO¥03-Aug-2004¥0¥¥# S
AC-CI(SACONLY, TARGETSTATE=(SPINSTATE=SINGLET,SYMMETRY=1,ROOT=0)) /D95
** OPT CPHF=CANONICAL TEST¥¥Gaussian Test Job 647 (Part 3): Geometry o
ptimization calculation of the SAC ground state of BH with full-valenc
e active MOs of D95**. Initial geometry is the experimental one.¥¥0,1¥
B,0.,0.,-0.2073863009¥H,0.,0.,1.0369315043¥¥Version=AI64T-G03RevC.02¥S
tate=1-SG¥HF=-25.1238297¥RMSD=8.923e-09¥RMSF=4.383e-08¥Dipole=0.,0.,0.
5838453¥PG=C*V [C*(H1B1)]¥¥@


SCIENCE AND PEACE WILL TRIUMPH OVER IGNORANCE AND WAR

                          -- PASTEUR
Job cpu time:  0 days  0 hours  0 minutes 19.6 seconds.
File lengths (MBytes):  RWF=     25 Int=      0 D2E=      0 Chk=     10 Scr=     58
Normal termination of Gaussian 03 at Tue Aug  3 13:37:06 2004.
```

Part VI. Frequently Asked Questions (FAQ)

VI-A. List of FAQ raised about the SAC-CI method

1. How to start the SAC-CI calculations

Q. What can I study with the SAC-CI program on Gaussian 03?

Q. Learning the SAC-CI method: methodology and computations.

Q. Are there sample inputs for the SAC-CI calculations?

Q. How to determine number of solution in each symmetry?

2. Choice of Basis sets in the SAC-CI calculations

Q. Valence and Rydberg states of organic aromatic compounds

Q. Excited and ionized states of the porphyrin compounds

Q. Excited and ionized states of ethylene

Q. Excited states of transition metal complexes

Q. Shake-up ionized states in valence ionization spectra

Q. Core-electron excitation and ionization

Q. Metal surfaces

Q. Geometry optimization of large molecules

Q. Hyperfine splitting constants

3. Method and Accuracy

Q. Levels of accuracy in the SAC/SAC-CI calculations

Q. How to set the threshold for the selection?

Q. Dimension (number of the excitation operators) of the SAC/SAC-CI calculations

Q. What is the default in SAC-CI calculation?

Q. What is the difference between EOM-CC, CC-LRT, and SAC-CI?

Q. How to calculate the ground and excited states of molecules having open-shell ground state? With ionization or with electron-attachment?

Q. Is it possible to calculate the excited states of species with a triplet spin ground state, e.g. oxygen atom or oxygen molecule, and what does the input look like?

Q. Is it possible to calculate the bond energies, A-B → A + B (A, B: radical) using the SAC/SAC-CI method with the following procedure?

4. Large system

Q. Job terminates at integral transformation (Overlay8) due to full of disk space.

Q. Job terminates with "No memory left for SECI diagonalization". I specified

“MaxR2Op=100000000”.

Q. Perturbation selection takes time and the job does not proceed.

Q. In the step "PRES", the job terminates with the message,"the Number of R2 operators is larger than ...".

Q. How to determine the memory size with the option “%mem” for SAC-CI calculation?

Q. In calculations with large active space. the calculation takes very long time to diagonalize the reference-CI matrix.

Q. Save core-memory by using Real*4 MO ERI (Electron Repulsion Integrals) in instead of the Real*8 one.

5. Potential energy surface

Q. Does the selection of the operators affect the smoothness of the potential surface?

Q. Potential curve for single-bond twisting.

6. Geometry optimization

Q. Initial geometry for the SAC-CI optimization

Q. Should I use geometry optimized by the SAC method for calculations of the vertical excitation energy with the SAC-CI method?

Q. MOs during the geometry optimization

Q. Number of solutions in the SAC-CI optimization

Q. PES and vibrational frequency calculations

Q. Is the MOD method dependent on the initial structure?

Q. Geometry optimization terminated at step “ZVECIT”.

Q. How to check the convergence behavior in the SAC-CI optimization?

Q. How can we check the MOD method work properly?

Q. In a frequency calculation, large force (larger than the convergence threshold) was calculated. I have optimized the molecular geometry with SAC/SAC-CI method and the optimized geometry was used for the frequency calculation.

7. General-*R*

Q. When do we use the SAC-CI general-*R* method?

Q. How to generate the higher-order linked operators in the SAC-CI general-*R* calculations

Q. What are the reference state and the active space for the perturbation selection in the general-*R*?

Q. How to determine the thresholds for the exponential generation of the higher-order excitation operators?

8. Core-electron excitations and ionizations

Q. Is there sample input for calculating core-electron processes?

Q. Why Rydberg basis sets are necessary in core-electron excitations and ionizations

9. Relativistic effect

Q. How I can include the scalar relativistic effect into SAC-CI calculations?

Q. Spin-Orbit interaction included in the SAC-CI states as the first-order perturbation.

10. Property

Q. Sign of transition moment changes

Q. Can I calculate transition moment between the excited states?

Q. Is the SAC-CI method applicable to Circular Dichroism (CD) spectrum?

Q. Can we calculate the electrostatic properties with the SAC-CI relaxed density matrix?

Q. How to study hyperfine splitting constants (hfsc) with the SAC-CI method.

11. Other questions

Q. Is there explanation about the SAC-CI output?

Q. How can we understand the SAC-CI wave function in the output?

Q. What is the definition of the excitation energy? Is it the relative energy from the SAC state (closed-shell singlet state) or the lowest state in each spin-symmetry?

Q. Which kind of computational resources is necessary to perform SAC-CI calculations?

Q. Job terminates at generating the initial guess orbitals (Overlay4).

VI-B Answers to the questions

1. How to start the SAC-CI calculations

Q. What can I study with the SAC-CI program on Gaussian 03?

A. SAC-CI program on Gaussian03 can calculate the ground and excited states of singlet, triplet, ionized, electron-attached, and other higher spin multiplicities. The program also calculates energy gradient of these states, which is force acting on nuclei. Using the SAC and SAC-CI wave functions, various one-electron properties and transition properties are also available. The range of the applications spreads into many research fields in physics and chemistry. In the SAC-CI guide, a part of the application is explained with sample inputs.

SAC-CI program (Nakatsuji 1985)

SAC method

- **Singlet closed shell ground state**

SAC-CI method

- **Singlet excited states**
- **Triplet states**
- **Ionized doublet states**
- **Electron attached doublet states**
- **High-spin(Quartet-Septet states)**

Analytical energy gradient

Applicable to Physics and Chemistry in these states

Q. Learning the SAC-CI method: methodology and computations.

A. We first recommend looking at SAC-CI guide which is available via the web site http://www.sbchem.kyoto-u.ac.jp/nakatsuji-lab

To start SAC-CI calculation, it is recommended to start with test631.com, in which one can compare the SAC-CI and full-CI results for the excited, ionized, and electron-attached states of H_2O with double-zeta basis.

Q. Are there sample inputs for the SAC-CI calculations?

A. Yes, users can refer to sample inputs $g03root/g03/tests/com/test631.com ~ test675.com, test689.com. These inputs show typical scientific problems.

Single point calculations for the excited, ionized, electron-attached, and high-spin states: test631~ test636

Free Base Porphin: test637

Geometry optimization: test638, test639

Use of LMO (Localized Molecular Orbital): test642

GSUM (Group SUM of the excitation operators): test644

General-R method: test646, test647, test667

Q. How to determine number of solution in each symmetry?

A. It is better to perform a preliminary calculation before the final calculations. There are several prescriptions.

1. Use of CIS result: The SD-*R* calculation uses CIS states for the reference state in the perturbation selection. Since CIS results provide qualitative picture, you can determine how many solutions are necessary to obtain the state of interest. In the SAC-CI keyword, "SelectCISOnly" option stops the calculation after the CIS diagonalization and the selection of operators.

2. Use of "NoSymmetry" keyword (non SAC-CI option): This option abandons use of symmetry in the calculations. Specify seemingly enough number of solutions and perform SAC-CI calculation with the "NoSymmetry" option and low-level threshold for the perturbation selection. Looking at the MOs, one can easily find symmetry of MOs and hence symmetry of the excited states. Finally, you determine number of solutions in each irreducible representation. With the use of symmetry, you can perform fine calculation with the much better threshold.

2. Choice of Basis sets in the SAC-CI calculations

Q. Valence and Rydberg states of organic aromatic compounds

A. For substituted benzenes such as aniline or *p*-benzoquinone, the basis sets we used were Huzinaga-Dunning's (9*s*5*p*/4*s*)/[5*s*3*p*/3*s*] with standard scaling factors plus Huzinaga's polarization functions([2*d*] for C, N and O, [1*p*] for H), Dunning's diffuse anion basis ([1*s*1*p*] for C, [2*s*2*p*] for N, O) split with the standard splitting factors. They were augmented with Dunning's Rydberg functions (3s, 3p, and 3d functions of carbon split into [2s2p2d] with standard splitting factors) at

the center of the molecule. (See J. Phys. Chem. A., 106, 3838-3849 (2002) for p-benzoquinone and J. Chem. Phys., 117, 2045-2052 (2002) for aniline.)

For five-membered ring compounds such as furan, pyrrole and thiophen, or azabenzene such as pyridine, we used Dunning's augmented correlation consistent polarized triple zeta basis sets, AUG-cc-pVTZ, for O, N, S and C atoms with one *f* polarization function removed for all C atoms, and cc-pVTZ for H atoms. Additionally, a set of diffuse functions (5*s*5*p*5*d*) were placed on the molecular center of gravity to investigate the Rydberg states in a wide energy region. (See J. Chem. Phys., 113, 7853-7866 (2000) for furan and pyrolle, J. Chem. Phys., 114, 842-850 (2001) for thiophen, and J. Chem. Phys., 114, 5117-5123 (2001) for pyridine.)

Q. Excited and ionized states of the porphyrin compounds

A. To calculate the absorption spectrum of porphyrin compounds, we recommend at least valence double-zeta plus polarization d-functions on C and N atoms. However, the effect of polarization function was not so significant in the low-lying singlet excited states. See our previous study published in J. Phys. Chem. A 102(10), 1843-1849 (1998). For calculating the ionized states, we recommend including the polarization d-functions on C and N atoms.

Q. Excited and ionized states of ethylene

A. For the valence excited states and ionized states, a recommended basis sets is the triple-zeta and polarization d-function for the C atoms, and the double-zeta and polarization p-function for the H atoms. These basis sets are augmented with Rydberg s and p set on carbons and two diffuse d-functions on the center of the bond.

For calculating Rydberg states, at least additional s and p type Rydberg functions should be included. See test634 and its description in the Part-I-L of the SAC-CI guide. See also previous articles

H. Nakatsuji, J. Chem. Phys. 80 (1984) 3703.

C.C. Ballard, M. Hada, and H. Nakatsuji, Bull. Chem. Soc. Jpn. 69 (1996) 1901.

J. Hasegawa, M. Ehara, and H. Nakatsuji, Chem. Phys. 230 (1998) 23.

Q. Excited states of transition metal complexes

A. In our experiences, the following basis sets work very nicely for the excited states of tetraoxo-transition metal complexes and photochemistry of $Ni(CO)_4$. Our recommendation is the valence double-zeta set plus double polarization p-function for the central metal and the double-zeta set for the ligand atoms. In $Ni(CO)_4$, [6s2p2d/4s2p] set was augmented with double polarization p-function for the Ni atom and with Rydberg s and p functions for the C and O atoms (J. Chem. Phys. 103, 6993-6998 (1995)). In TcO_4^{2-}, [7s3p3d/4s2p] set was augmented with double polarization p-function for the Tc atom (Theoret. Chim. Acta, 92, 351-359 (1995)). Please find more details in the original papers and the references therein. Use of ECP is not recommended (J. Chem. Phys., 97, 2561-2570 (1992)).

Q. Shake-up ionized states in valence ionization spectra

A. Polarization functions are important for calculating ionized states, and the Rydberg basis sets are also necessary for describing the shake-up states converging to the double ionization threshold. The valence triple zeta with double polarization functions plus some Rydberg functions are recommended. See, for example, J. Chem. Phys. 114, 8990 (2001).

Q. Core-electron excitation and ionization

A. The basis sets should be flexible enough to describe orbital reorganizations and electron correlations. The polarization functions of inner-shell orbital, first derivatives of 1s functions, i.e. p-type functions, are necessary for describing the polarizations and the angular correlations of the 1s electrons. See, for example, J. Chem. Phys. 122, 014304 (2005).

Q. Metal surfaces

A. The basis sets for the adsorbed molecules could be triple zeta level, and those of the metal surface could be ECP(effective core potential) and the double-zeta level. See for example, J. Chem. Theory Comput., 1 (2), 239 -247, 2005.

Q. Geometry optimization of large molecules

A. The double-zeta polarization basis sets would be the smallest sets having acceptable accuracy. The correlated methods such as SAC-CI method have to calculate so-called one-body and two-body effective density matrices (EDM) to compute the energy gradient of a state. The EDMs are first calculated in the MO basis and transformed into the AO basis. This back-transformation is one of the time-consuming steps in the gradient calculations, and the transformation can be quickly done when the AO dimension is smaller. One may chose the valence double-zeta sets instead of the double-zera sets, because the AO dimension is smaller and the accuracy of the geometry is not so different.

Q. Hyperfine splitting constants

A. The basis sets should be double or triple zeta quality for describing K-shell orbital, augmented with polarization functions. The STO-GTO expansion method is useful for including the cusp condition of the wave function at nucleus. (See, J. Chem. Phys. 91, 6205 (1989))

3. Method and Accuracy

Q. Levels of accuracy in the SAC/SAC-CI calculations

A. Levels of accuracy can be controlled by the options LevelOne / LevelTwo / LevelThree, which are in order of increasing the accuracy. These define energy thresholds for the perturbation selection of linked double-excitation operators in the SAC/SAC-CI wave functions. LevelThree is set as the default. In LevelOne, EThreS2=1*10**(-5), EThreR2=1*10**(-6) a.u., in LevelTwo, EThreS2=5*10**(-6), EThreR2=5*10**(-7) a.u., and in LevelThree, EThreS2=1*10**(-6), EThreR2=1*10**(-7) a.u..

Q. How to set the threshold for the selection?

A. We recommend LevelThree (default) for the final calculation. Lower level calculations become more approximate. Even though the LevelOne results are quantitative enough, the reliability of the result should be carefully examined.

Q. Dimension (number of the excitation operators) of the SAC/SAC-CI calculations

A. Dimension of the SAC/SAC-CI calculations, number of the excitation operators, depends on the threshold of the perturbation selection, LevelOne / LevelTwo / LevelThree. Before doing the whole SAC-CI calculations, one can check the size of the calculations by using the option "SelecCISonly". We note that a calculation more than 400,000 linked operators would take more than a week in ordinary work stations (for example, HP DS25/alpha 1.0GHz). To reduce the dimension, you can try the lower level of selection or reduce number of solution in the SAC-CI calculation

Q. What is the default in SAC-CI calculation?

A. When no options are given, the program executes SAC-CI SD-*R* calculation for singlet, triplet, and ionized states with one solution for each symmetry. Default actions of the SAC-CI program are summarized in the "I-H-3 summary of the keywords and the default action" of SAC-CI GUIDE.

Q. What is the difference between EOM-CC, CC-LRT, and SAC-CI?

A. The EOM-CC(1989,1993)[1] and the CC-LRT methods(1979,1990)[2] are theoretically equivalent to the SAC-CI method(1978). Some numerical proofs showing the equivalence of these methods are given in the "I-E. Equivalence of EOM-CC and CC-LRT to SAC-CI" of SAC-CI GUIDE. We performed the SAC-CI SD-*R* calculations for CH_2 and CH^+ for which the EOM-CCSD[4] and CCSD-LRT[5] calculations were reported. We also show that the approximation of neglecting the unimportant unlinked terms and the perturbation selection of the linked operators are both accurate and useful. It should be noted that the program system MEG/EX-MEG[6] coded in 1985 can perform both SAC-CI SD-*R* and general-*R* calculations as special cases of more general MEG/EX-MEG calculations [7-10] without introducing any approximations.

A policy of the SAC/SAC-CI program is that we calculate only important terms, and we neglect terms if their effect are certainly negligibly small. By doing so, we can make the computations more efficient, so that we can calculate larger and more complex systems, and the physics and chemistry of the calculated results become clearer than otherwise. It is by this virtue that we could have been able to apply our SAC-CI method to the porphyrin systems and to the reaction center of photosynthesis of *Rhodopseudomonas viridis*. For this purpose, we may introduce the following approximations. (1) Some classes of unimportant unlinked terms are neglected from the beginning. (2) The perturbation selection of the linked operators and further the selection among the unlinked terms composed of the selected linked terms are performed.

[1] J.Geertsen, M. Rittby, R. J. Batlett, Chem. Phys. Lett. 164, 57 (1989); J.F. Stanton and R.J.

Bartlett, J. Chem. Phys. 98, 7029 (1993).
[2] D. Mukherjee and P.K. Mukherjee, Chem. Phys. 39, 325 (1979); H. Koch and P. Jorgensen, J. Chem. Phys. 93, 3333 (1990).
[3] H. Nakatsuji, Chem. Phys. Lett., 59, 362 (1978); ibid, 67, 329, 334 (1979).
[4] S. Hirata, M. Nooijen, R.J. Bartlett Chem. Phys. Lett. 326, 255 (2000).
[5] H. Koch, H. J. Aa. Jensen, P. Jorgensen, T. Helgaker, J. Chem. Phys. 93, 3345 (1990).
[6] H. Nakatsuji, Program system for the MEG/EX-MEG methods applied molecluar ground, excited, ionized and electron attached states, 1985.
[7] H. Nakatsuji, J. Chem. Phys. 83, 713, 5743 (1985).
[8] H. Nakatsuji, Theoret. Chim. Acta, 71, 201 (1987).
[9] H. Nakatsuji, J. Chem. Phys. 94, 6716 (1991).
[10]H. Nakatsuji, J. Chem. Phys. 95, 4296 (1991).

Q. How to calculate the ground and excited states of molecules having open-shell ground state? With ionization or with electron-attachment?

A. There are four approaches for calculating open-shell systems depending on the choice of the reference orbitals and the operators used in the SAC-CI wave function.

Case 1: ROHF SCF (N) – SAC (N+1) – SAC-CI, CationDoublet (N)

Case 2: ROHF SCF (N) – SAC (N-1) – SAC-CI, AnionDoublet (N)

Case 3: RHF of Cation (N-1) – SAC (N-1) – SAC-CI, AnionDoublet (N)

Case 4: RHF of Anion (N+1) – SAC (N+1) – SAC-CI, CationDoublet (N)

where (N), (N-1) and (N+1) denotes the number of electrons. Since these types of calculations give almost the same results, we do not have special recommendation. We can choose the reference orbitals by specifying the charge and the multiplicity just one line above the “Gaussaian molecular specification”. The choice “CationDoublet” or “AnionDoublet” should be specified in the SAC-CI part of input.

As described above, there are two ways to construct the open-shell ground-state wave function by the SAC-CI method: via CationDoublet (1 and 4) or AnionDoublet (2 and 3). The former removes one electron from the (N+1)-electron closed-shell SAC wave function, and the latter attaches one electron to the (N-1)-electron closed shell SAC wave function. Therefore, the way to obtain the excited states is different in these two cases.

In the molecules having the open-shell ground-state, we can classify the one-electron excited states into three.

Case A: Excitation from the doubly occupied MOs to SOMO

Case B: Excitation from the SOMO to the unoccupied MO

Case C: Excitation from the doubly occupied MOs to the unoccupied MO

We note here that even such one-electron excited states should be treated as a two-electron process in the SAC-CI calculation, because of the open-shell ground state. In the “CationDoublet” (1 and 4) case, the wave function of the case A can be described by one-electron ionization from the SAC state having (N+1)-electrons. Cases B and C, however, should be described by two-electron

process: one-electron ionization and one-electron excitation. In the “AnionDoublet” (2 and 3) case, only case B can be described by one-electron attachment to the SAC state having (N+1)-electrons. The cases A and C should be described by two-electron process: one-electron attachment and one-electron excitation.

One-electron process from the SAC closed-shell state can be treated by the SAC-CI SD-*R* method, while two-electron process from the closed-shell state requires SAC-CI general-*R* method. In closing, we give a Table to summarize the above discussion.

Table. SAC-CI approach to the excited state for the open-shell ground state molecules.

		Construction of the open-shell ground-state wave function			
		Case 1	Case 2	Case 3	Case 4
Type of the excited states	Case A	One-elec. process (SD-*R*)	Two-elec. process (general-*R*)	Two-elec. process (general-*R*)	One-elec. process (SD-*R*)
	Case B	Two-elec. process (general-*R*)	One-elec. process (SD-*R*)	One-elec. process (SD-*R*)	Two-elec. process (general-*R*)
	Case C	Two-elec. process (general-*R*)	Two-elec. process (general-*R*)	Two-elec. process (general-*R*)	Two-elec. process (general-*R*)

Q. Is it possible to calculate the excited states of species with a triplet spin ground state, e.g. oxygen atom or oxygen molecule, and what does the input look like?

A. It is possible to calculate triplet ground state with SAC-CI method. However, since the current SAC-CI program starts with the calculation of the closed shell SAC state, the accuracy of the calculation for molecules like O_2 depends on how one defines the closed-shell state. The accuracy can be improved if you include higher-excited operators in the SAC-CI general-*R* method.

Q. Is it possible to calculate the bond energies, A-B → A + B (A, B: radical) using the SAC/SAC-CI method with the following procedure?

1) The SAC calculation for the closed shell molecule A-B

2) The SAC-CI calculations for the radicals A and B

3) (Bond energy) = (SAC-CI energy of A) + (SAC-CI energy of B) – (SAC energy of A-B).

A. The calculation is possible in principle. The results would be reliable if the keywords “NolinkedSelection” and “NoUnlinkedSelection” are used. We do not recommend such calculations, because of the computational cost. Instead, we suggest considering whether the GSUM method is applicable to your system.

4. Large system

Q. Job terminates at integral transformation (Overlay8) due to full of disk space.

A. When large active space is specified, overlay8 automatically uses large disk space and the calculation terminates when the read-write file exceeds the limit of disk space. In this case, user can declare the available disk space with "Maxdisk" option.

Q. Job terminates with “No memory left for SECI diagonalization”. I specified “MaxR2Op=100000000”.

A. This error message indicates the memory shortage at the SECI diagonalization step. The reason would be in the option, "MaxR2Op=100000000". This is too large. A recommended value would be at most 500000.

In addition, you can use "RefCIWindow" option in the SAC-CI keyword. This specifies the active orbitals in the SECI calculation. The SECI solution is used as the reference state for the perturbation selection of 2-electron excitation operators in the SAC-CI calculation. Therefore, the SECI active space is not necessarily equal to the SAC-CI active space.

Q. Perturbation selection takes time and the job does not proceed.

A. For the system with large active space, perturbation selection usually takes much cpu time. It does not mean that the calculation is in trouble. For example, the calculation with the active space of 330 MOs takes about two weeks for selecting the *S* and *R* operators in the step "PRES" with Compaq XP1000 workstation. Better algorithm has been developed and will be published soon..

Q. In the step "PRES", the job terminates with the message,"the Number of R2 operators is larger than ...".

A. For particularly large calculations, the number of the selected configuration may exceed the default value (100000), and the job terminates with the message of "the Number of R2 operators is larger than ...". In this case, user can avoid this problem by the following three options;

(1) Increase “MaxR2Op” option up to the required number of configurations,

(2) Decrease the level of accuracy (LevelThree / LevelTwo / LevelOne), to reduce number of the selected R2 operators, and

(3) Decrease number of solutions, if it is unnecessarily large.

Q. How to determine the memory size with the option “%mem” for SAC-CI calculation?

A. To achieve good performance in the SAC/SAC-CI, it is recommended to use appropriate memory size for the system. In SAC/SAC-CI, MOERIs (MO Electron Repulsion Integrals) are stored “in-core” for fast random accesses in calculating Hamiltonian matrix elements. Since the MOERI usually dominates the core memory in the large systems, the following remarks may be informative.

(1) ERIs that are zero due to the symmetry are automatically omitted.

(2) When the size of the ERIs is larger than the core memory of a computer, a bucket-type algorithm is adopted, which is effective only for the SD-*R* part. For details, see explanation in #SDPRES# in the SAC-CI guide.

(3) The size of ERIs stored in core is approximately 8*(N*(N-1)/2)/Nrep words, where N=Nact*(Nact-1)/2, Nact is the active space of SAC/SAC-CI and Nrep is the number of irreducible symmetry representation. Memory size should be increased using %MEM or -M-, in large

calculations, especially when the message “Recommend to increase core memory” appears.

Q. In calculations with large active space. the calculation takes very long time to diagonalize the reference-CI matrix.

A. This is because the reference-CI uses in-core diagonalization. In such cases, we recommend to use RefCIWindow option to reduce the active space for the reference CI calculation.

Q. Save core-memory by using Real*4 MO ERI (Electron Repulsion Integrals) in instead of the Real*8 one.

A. The SAC-CI program treats the MOERI in core memory. This means that we can perform larger systems if we can save the size of the MOERI. One way is to reduce the accuracy of the MOERI from Real*8 to Real*4. This reduction allows us to treat the active space by 1.2 times larger than the real*8 case. The result of the calculations does not show any meaningful changes as shown in the appendix of the SAC-CI guide.

To generate the Real*4 executable (l923.exe), one can include USE_R4 option as an option for executing cpp. In alpha-osf1 case, include “-DUSE_R4” as a part of “ALPHADEF” in “alpha-osf1.make”.

5. Potential energy surface

Q. Does the selection of the operators affect the smoothness of the potential surface?

A. To calculate large molecules, the SAC-CI program performs the perturbation selection of the excitation operators. The set of the selected operators depends on the geometry. This dependency can affect the smoothness of the potential surface, when the low-level threshold was used for the selection. We note that the calculated potential surface is rather smooth, and the vibrational frequency become very close to the experiments, when the high-level selection was performed.

We recommend using GSUM (Group SUM of the excitation operators) method for calculating the potential surface. The GSUM method takes group sum of the operators selected at different geometries, and the final set of the excitation operators are qualitatively equivalent in all of the examined geometries. Please find some descriptions in the SAC-CI guide. We also provided a sample input for the GSUM calculations in test644.

Q. Potential curve for single-bond twisting.

A. Twisting single-bonds sometimes induce large change in the amplitude of the canonical MOs. In such situations, one to one correspondence between MOs in the neighboring geometry become worse and this affects the accuracy of the GSUM calculations.

We recommend using LMO in the GSUM calculation for the twisting single-bond, because LMO is much more independent on the geometry of the molecules.

6. Geometry optimization

Q. Initial geometry for the SAC-CI optimization

A. SAC-CI geometry optimization uses Minimum Orbital Deformation (MOD) method (See details in the SAC-CI guide). Since the MOD method uses the MOs at the initial geometry as the reference

orbitals, this could induce the initial-structure dependence in the optimized structure. Therefore, the initial geometry for the optimization is better to be close to the optimized structure. We provided MacroIteration option which allows repeating the optimization starting from the optimized geometry in the previous cycle. This option reduces such initial geometry dependence.

Q. Should I use geometry optimized by the SAC method for calculations of the vertical excitation energy with the SAC-CI method?

A. Using the optimized geometry with the SAC method is of course a good choice for the calculations of vertical excited states. However, the geometry optimization with the SAC method is costly and practically impossible for large molecules. You can use experimental or optimized geometry with less expensive method, if those geometries are enough accuracy. For further details, refer to our articles.

Q. MOs during the geometry optimization

A. MOs printed out at the end of the job using "pop=full" may differ from those for the initial geometry in the SAC-CI geometry optimization. For analyzing the nature of the excited state, it is recommended to perform single point SAC-CI calculation at the converged optimized geometry. This is automatically done by "MacroIteration=1".

During geometry optimization, MOD (Minimum-Orbital-Deformation) algorithm is performed in order to obtain continuous orbital nature during the optimization. In other words, canonical MOs are not used in the optimization process.

Q. Number of solutions in the SAC-CI optimization

A. Users can calculate other excited states in the SAC-CI goemetry optimization. The reference states in the perturbation selection are chosen by referring to the requested number of solutions. For example, following input calculates three roots for symmetry 3 and the geometry optimization is done for the second state. In this case, operators are selected with the three reference states.

```
#SAC-CI=(Triplet=(NState=(0,0,3,0)),
TargetState=(SpinState=Triplet, Symmetry=3, Root=2))/D95 Opt
```

When users are interested in only the optimized state, it is efficient to specify the mimimum number of solutions; namely, in the above case, Triplet=(NState=(0,0,2,0)).

With the input of Triplet=(NState=2), users can calculates other space symmetry like A_1, A_2, and B_2 states in C_{2v} group.

Q. PES and Vibrational frequency calculations

A. In the present version of the SAC-CI method, the harmonic frequency can be calculated in combination with the GSUM method. An example is given as test689.com. In the GSUM step, the sample geometry should include the stationary point.

GSUM method is very important for calculating potential energy curves. Please refer to SAC-CI Guide for details and test644 which calculates the potential energy curves of Li_2. For calculating reliable harmonic frequency and anharmonic frequency, the GSUM method is strongly recommended.

Q. Is the MOD method dependent on the initial structure?

A. When the MOD method is used, the pertubation selection is not performed during the optimization; the *S* and *R* operators selected at the initial geometry are used. Therefore, the suitable initial geometry should be used. We can confirm the optimized structure by "MacroITer" option, in which optimization is iteratively performed with the converged structure.

Q. Geometry optimization terminated at step "ZVECIT".

A. There are two possible solutions.

1) Change the convergence threshold of SAC-CI diagonalization with the input of "DConvDiag=6".

2) Change the cutoff parameter with the input of "CutoffDIISZVec=1.0d-3". See test648.com

Q. How to check the convergence behavior in the SAC-CI optimization?

A. Please check the total energy and force at each iteration of the optimization. It is convenient to check the lines including the following expresstions.

ECorr(SAC-CI-V)= … Total energy= …

Cartesian Forces: Max … RMS …

When the convergence of total energy is oscillating, please perform the single point calculation. Examine whether there are other excited states lying near the target state. It happens that the character of the target state exchanges due to such close lying excited states.

Q. How can we check the MOD method work properly?

A. Please check the "Overlap analysis" at "Transform orbitals by the MOD method".

"Min eigenvalue" should be close to one and others should be almost zero.

Q. In a frequency calculation, large force (larger than the convergence threshold) was calculated. I have optimized the molecular geometry with SAC/SAC-CI method and the optimized geometry was used for the frequency calculation.

A. Use the larger number of "Macroiteration" for the geometry optimization. The GSUM method has to be used in the frequency calculations. See test689.com for a sample input.

7. General-*R*

Q. When do we use the SAC-CI general-*R* method?

A. The SAC-CI SD-*R* method is appropriate for ordinary single-electron excitation, ionization, and electron-attachment processes. In the SAC-CI general-*R* method, the order of the excitations operator is generalized upto higher-order excitations. Current SAC-CI program can include the

excitation operators (*R*-operators) upto sextuple excitations. The general-*R* method is appropriate for multi-electron processes like two-electron excited states and shake-up ionizations.

Q. How to generate the higher-order linked operators in the SAC-CI general-*R* calculations

A. The higher-order (more-than-triple) linked operators are generated by the exponential generation algorithm in the single point energy calculation by default. The highest *R* is specified by MaxR(<=6).

"FullRGeneration" option requests to generate all higher-order linked operators in general-*R* with MaxR<=4 and then to perform perturbation selection.

Q. What are the reference state and the active space for the perturbation selection in the general-*R*?

A. In the default general-*R* calculations, SDCI solutions are used for the reference states of the perturbation selection. This reference SDCI is performed with a small active space and diagonalized by in-core algorithm.

The size of the active space in the SD-CI is automatically determined, according to the memory size and the orbital energies. User can specify the active space with "RefCIWindow" option. However, when the estimated SDCI dimension for each symmetry exceeds 2000, the active space is reduced regardless of the memory size. If users want to specify this small active space for large reference SDCI dimension, "Namelist" option should be used as follows.

```
# SAC-CI(…, Namelist)

 &ghpres mxdiag=5000, &End
```

where the maximum dimension of 5000 is specified.

Q. How to determine the thresholds for the exponential generation of the higher-order excitation operators?

A. Higher-order linked excitation operators up to sextuples are generated by the exponential generation scheme described in the following papers:

H. Nakatsuji, Chem. Phys. Letters, 177, 331 (1991).

H. Nakatsuji, J. Chem. Phys. 83, 713, 5743 (1985).

H. Nakatsuji, J. Chem. Phys. 94, 6716 (1991).

See also description about EGOP in the Part II-C of the SAC-CI guide. Single excitation operators are included without selection. Doubles are handled as in SD-*R* part of the program. Higher-order excitation operators are generated as the products of A and B operators, R=A*B, A*A*B. The A and B operators are single and double excitation operators and selected with a criterion explained below.

The second-order product generates triple and quadruple excitation operators.

R=A(S)*B(D) and A(D)*B(S), triples

A(D)*B(D) quadruples

"S" and "D" denote single and double excitation operators, respectively. The A-operators used for the second-order products are single and double excitation operators whose coefficients in the reference SD-CI wave function are larger than given thresholds

CThreEgABAOp=(A1Op=<thrma1>,A2Op=<thrma2>).

The <thrma1> and <thrma2> are thresholds for the single and double excitation operators, respectively.

The third-order product generates quintuple and sextuple excitation operators.

R=A(D)*A(D)*B(S) and A(D)*A(S)*B(D), quintuples

A(D)*B(D)*B(D) sextuples

The A-operators used for the third-order product are also single and double excitation operators whose coefficients in the reference SD-CI wave function are larger than given thresholds

CThreEgAABAOp= (A1Op=<thmma1>,A2Op=<thmma2>).

The <thmma1> and <thmma2> are thresholds for the single and double excitation operators, respectively.

For B-operators, the thresholds are given by

CThreEgAB=(B1Op=<thrmb1>,B2Op=<thrmb2>) for the second-order product and

CThreEgAAB=(B1Op=<thmmb1>,B2Op=<thmmb2>) for the third-order product.

The <thrmb1> and <thmmb1> are thresholds for the single excitation operators, and the <thrmb2> and <thmmb2> are those for the double excitation operators.

Thus, the accuracy of the exponential generation of the higher *R* operators in the general-*R* method is expressed by a set of the thresholds,

(<thrma1>, <thrma2>, <thmma1>, <thmma2>) and

(<thrmb1>, <thrmb2>, <thmmb1>, <thmmb2>).

The default values are

(<thrma1>, <thrma2>, <thmma1>, <thmma2>)=(0.04, 0.04, 0.1, 0.1)

(<thrmb1>, <thrmb2>, <thmmb1>, <thmmb2>).=(0.04, 0.04, 0.1, 0.1)

These parameters can be defined for each spatial- (ISYM) and spin-symmetries (KSTATE). In addition, the linked operators up to quadruple are further filtered by the perturbation selection with a given threshold (EThreEgR or eseleg). For quintuple and sextuple excitation operators, no perturbation selection is performed.

8. Core-electron excitations and ionizations

Q. Is there sample input for calculating core-electron processes?

A. There are sample inputs for calculating the K-shell ionization potential, geometry, and shake-up satellite spectra of H_2O. (They are not included in the current distributed version of G03.)

Q. Why Rydberg basis sets are necessary in core-electron excitations and ionizations

A. Since Rydberg states appear in the energy range similar to the valence states, it is quite natural that Rydberg states appears in the core-electron process as the many-electron processes. For

example, in the satellite peaks related to the core-electron ionizations, the electronic structure of the states may involve two electron processes: one-electron core-ionization and one-electron Rydberg excitation.

9. Relativistic effect

Q. How I can include the scalar relativistic effect into SAC-CI calculations?

A. Gaussian03 provides several kinds of the scalar relativistic integrals. They can be combined to the SAC-CI calculations.

Q. Spin-Orbit interaction included in the SAC-CI states as the first-order perturbation.

A. The spin-orbit interaction can not be considered with the current program. The spin-orbit interaction can be included with the quasi-degenerate perturbation method for the SAC/SAC-CI wave functions. For further details, refer to our previous studies.

H. Nakatsuji, Y. Matsuzaki, and T. Yonezawa, J. Chem. Phys., 88(9), 5759-5769 (1988).

H. Nakatsuji and M. Ehara, J. Chem. Phys., 101(9), 7658-7671 (1994).

10. Property

Q. Sign of transition moment changes

A. The sign of the wave function is arbitrary, and therefore, the sign of the transition moment is also arbitrary. The sign is dependent on MOs, convergence, and machines. Oscillator strength can be compared with the intensity of the experimental spectrum.

Q. Can I calculate transition moment between the excited states?

A. Yes. Include TransitionFrom option which specifies the initial state of the transition.

Q. Is the SAC-CI method applicable to Circular Dichroism (CD) spectrum?

A. Yes. Rotational strength in the CD spectrum can be calculated with the SAC and SAC-CI wave function. See sample job.

Q. Can we calculate the electrostatic properties with the SAC-CI relaxed density matrix?

A. Please add “Density=Current Prop=EFG”.

Q. How to study hyperfine splitting constants (hfsc) with the SAC-CI method.

A. The basis sets should be double or triple zeta quality for describing K-shell orbital, augmented with polarization functions. The STO-GTO expansion method is useful for including the cusp condition of the wave function at nucleus. (See, J. Chem. Phys. 91, 6205 (1989))

All single and double excitation operators are included in the SAC-CI wave function, and the perturbatoin selection is not performed. This is to avoid selecting out the configurations that are necessary to calculate hfsc. Configurations important for properties are not necessarily give significant contributions to the correlation energy.

11. Other questions

Q. Is there explanation about the SAC-CI output?

A. See SAC-CI guide in the SAC-CI home page.

Q. How can we understand the SAC-CI wave function in the output?

A. The SAC-CI operators are defined as excitations, ionizations, and electron attachments from the closed-shell SAC reference function. In singlet case, the output looks like

```
Single excitation    5   6     0.70
Double excitation    5   6   4   7   0.31        5   7   4   6   -0.32
                     5   6   5   7   0.11
```

The output shows that a single excitation from the 5th to 6th MO has coefficient of 0.70. The double excitation from the 4th and 5th MOs to 6th and 7th MOs is also a main configuration.. In this case, the electrons in 5th and 6th MOs have a singlet-coupling, and the electrons in 4th and 7th MOs make another spin-coupling. The excitation operator “5 7 4 6” and “5 6 4 7” has the same spatial occupation, but different spin-coupling. The two configurations span complete spin space. See the SAC-CI guide for the details.

In the CationDoublet case, the output looks like

```
###  1-st  ###
 Single excitation    5    0.90
 Double excitation    5   6   4   0.17    4   6   5    -0.15
###  2-nd  ###
 Single excitation    4    0.86
 Double excitation    5   6   4   0.27    4   6   4    -0.12
```

In the first solution, the single excitation “5” means the ionization from 5th MO. The double excitation “5 6 4” stands for the singlet excitation from 5th to 6th MO and the ionization from 4th MO.

Q. What is the definition of the excitation energy ? Is it the relative energy from the SAC state (closed-shell singlet state) or the lowest state in each spin-symmetry?

A. The result of the diagonalization of the SAC-CI Hamiltonian matrix would be printed out as follows.

```
###   1-st  ###          ---   1st state in this spin multiplicity ---
     This state is being used for optimizations.
     Total energy       in au =    -137.984448
     Correlation energy in au =      -0.211509
     Excitation energy  in au =       0.067464    in eV =       1.835777
```

```
 *SINGLE EXCITATION
      8    9     0.95882          8   13    -0.20786
      7    9    -0.05952          4    9    -0.03690
```

Here, “Excitation energy” is the relative energy from the SAC state. The same is for the other spin multiplicities. On the other hand, you would have the result for the transition property of the singlet states as followings.

```
Transition dipole moment of   singlet state from SAC ground state
-------------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
-------------------------------------------------------------------------------
   A1         0      0.0          Excitations are from this state.
   A1         1     10.7545      0.0000      0.0000      0.6593      0.1145
   A1         2     19.1017      0.0000      0.0000     -0.7882      0.2907
   A2         1     10.7291      0.0000      0.0000      0.0000      0.0000
   A2         2     26.5243      0.0000      0.0000      0.0000      0.0000
   B1         1      8.5939      0.2738      0.0000      0.0000      0.0158
   B1         2     24.9801      0.0961      0.0000      0.0000      0.0056
   B2         1     13.2224      0.0000     -0.6270      0.0000      0.1273
   B2         2     15.9912      0.0000      1.1672      0.0000      0.5337
-------------------------------------------------------------------------------
```

As you see in the output, the excitation energy is calculated as the relative energy from the SAC ground state. However, for the other spin-multiplicities, the excitation energy is calculated from the energy of the lowest state in each spin-multiplicity. See an example shown below. The excitation energies of the double ionized states are calculated from the 1^2B_1 state which the lowest state within the SAC-CI result.

```
Transition dipole moment of   ionized state from symmetry B1     1-th state
-------------------------------------------------------------------------------
Symmetry  Solution Excitation     Transition dipole moment (au)      Osc.
                   energy (eV)       X           Y           Z       strength
-------------------------------------------------------------------------------
   A1         1      1.7771     -0.1919      0.0000      0.0000      0.0016
   A1         2     22.9129      0.2647      0.0000      0.0000      0.0393
   A1         3     27.5008      0.1943      0.0000      0.0000      0.0254
   B1         1      0.0          Excitations are from this state.
   B2         1      7.1924      0.0000      0.0000      0.0000      0.0000
-------------------------------------------------------------------------------
```

Q. Which kind of computational resources is necessary to perform SAC-CI calculations?

A. The current version of SAC-CI on G03 tries to store the MOERI (Election Repulsion Integral in Molecular Orbital base) in core memory. Therefore, it is preferable to have the core-memory as large as possible. In addition, the cache size is also important for quick calculations. When you perform very fine calculation with large number of excitation operators, the size of the read-write file could be very large. In this case, the disk I/O becomes bottleneck of the computation.

Q. Job terminates at generating the initial guess orbitals (Overlay4).

A. The problem sometimes occurs when diffuse functions are adopted. It is caused by the code of Harris functional. In this case, user can avoid this problem by using the keyword “Guess=Huckel” or “Guess=Core”.

Appendix I. Summary of Changes in SAC-CI program

Ap-I. Summary of changes between versions (Aug2002) and 040803

1. Acceleration of the perturbation selection step of the two-electron excitation operators for large-scale calculations

Computational algorithm for the perturbation selection has been improved in the SAC-CI SD-R part of the program (Link 923). Number of the operation count becomes proportional to $O(N^5)$ × (Number of the reference state), though it is difficult to estimate the number of the operation count of the previous algorithm. The routines still keep all the required MO integrals: (ia|jb) for the ground state, and (ij|ka) & (ia|bc) for the singlet, triplet, and ionized, electron-attached states. Here, indices i, j, k and a, b, c refer to occupied and unoccupied orbitals, respectively. The core memory required for the integrals is (O×V)×(O×V+1) /2 for the ground state and $\{(O^2+O)/2\times(O\times V)\}+\{V^2+V\}/2\times(O\times V)\}$ for the excited, ionized, electron-attached states. If the computer allows handling these integrals at a time in the memory, the program selects the new routines. If not, the conventional selection routines are used.

Table Ap-I-1 shows the CPU time. The system is a chromophore of Cyan Fluorescent Protein (CFP), $C_{15}H_{15}N_3O_2$ (C_1-symmetry). The basis sets of DZP level was used, and total 290 active orbitals (51occ. & 239 unocc.) were used in the SAC/SAC-CI calculation. The number of the reference states was 8 in the selection. The comparison shows that the CPU time was drastically reduced for singlet and triplet excited states. However, for the ionized and electron-attached states, it takes more CPU time than the previous routines. This is because the total number of the two-electron operators (before selection) is small enough for the previous routine to finish within a manageable CPU time. This result shows that the new routine performs better when the target system is large.

Table Ap-I-1. Timing data (CPU time). CFP, $C_{15}H_{15}N_3O_2$ (C_1), DZP, 1s frozen core & frozen virtual (51occ. & 239 unocc.), Number of solution is 8.

	CPU time (HP DS25)	
	Sorting	Selection
Singlet ground states		
Previous	–	3m 25s
Present	1m30s	48s
Singlet excited states		
Previous	–	1h 53m 10s
Present	1m38s	6m 7s
Triplet states		
Previous	–	6h 47m 53s
Present	1m37s	11m 48s
Ionized doublet states		
Previous	–	41s
Present	1m38s	1s
Electron-attached states		
Previous	–	54s
Present	1m37s	11s

2. Frozen-core approximation available in the SAC-CI energy gradient and geometry optimizations

In the former version, frozen-core approximation could not be used in the SAC-CI energy gradient and geometry optimization calculations. This was very bad. In the revised version, this is improved: we can do SAC-CI geometry optimization with the frozen core MOs using the MOD (Minimum-Orbital Deformation) algorithm. We set the calculations with the frozen core MOs as default and removed the restriction of the full active space adopted in the former version of G03. We modified the L1.F, L801.F, L1002.F, and L1111.F for this improvement: some subroutines of MOD have been moved to L1111 and IOp(78) of overlay10 assigned to MOD is now not used by L1002. These functions were unified to IOp(46) of overlay11.

The titles of the following sample inputs were changed accordingly: test638.com, test639.com, test647.com, test648.com, test649.com, test651.com, test654.com, test655.com, test656.com, test657.com, test659.com, test660.com, test661.com, test662.com, test663.com, tes689.com.

3. Timing data improved in the SAC-CI geometry optimization for large molecules

In Link1111, 2-particle Effective Density Matrix (EDM) is transformed from MO to AO basis. This transformation was a time-consuming routine in the gradient calculation, especially when we treat large active space. This is because the use of the core memory was not efficient, and the routine had to rely on the disk-based computations.

We have replaced new two routines in the subroutine SacGam. SaBTr1 and SaBTr2 handle the first- and second-half back-transformation, respectively. Until the first-half transformation finishes, we have to keep all the EDM in core, because of the EDM routines. However, after the first half-transformation, the intermediate sorting step in SaBTr2 requires $(N_{MO}\times(N_{MO}+1))/2$ of memory in the minimum case. The second-half transformation works best, if the core memory treats all the half-transformed integrals of the size, $\{(N_{AO}\times(N_{AO}+1))/2\}\times\{(N_{MO}\times(N_{MO}+1))/2\}$.

In Table Ap-I-2, the present timing data is compared to the previous one. The wall clock time and CPU time are reduced to 1/5 and 1/2 in the new routines, respectively.

Table Ap-I-2. Timing data (Energy gradient for the excited states of Free Base Porphin, DZ basis, Full active, LevelOne)

Back transformation	Before		**After**	
	Wall clock	CPU	Wall clock	CPU
	5 h 09 m 11 s	2 h 35 m 27 s	**1 h 14 m 06 s**	**1 h 01 m 07 s**

We further reduced timing data of the SAC-CI geometry optimization. In the previous SAC-CI code (g03 ver. B04), we used subroutine SimEqn for solving the CP-MOD equations. This routine was computer-time demanding, when the dimension of the matrix was large. We included a new routine ModLin for iteratively solving the equation with much less computing time and core memory. In table Ap-I-3, we show the timing data of the geometry optimization for the first-excited state of free-base porphin. The data I show 8 hours of reduction in the single step. This is because the frozen-core approximation and the new back-transformation routine were introduced. As data II shows, further 2 hours of reduction has been achieved by the present development.

Finally, the SAC-CI geometry optimizations has been much accelerated: for free-base porphin, total real time 53 h (data 0) of the released version of G03 was reduced to 11h 37m (data II) in the present version. It is almost 1/5 of the previous one.

Table Ap-I-3. Improved computation time in the geometry optimization for the first-excited state of free-base porphin.[a]

	g03 ver. B04[b]	g03 ver. B07	
	0	I[c]	**II[d]**
L1111	7h 13m 21s	4h 25m 29s	**2h 09m 15s**
L1002	3h 59m 30s	4m 04s	**4m 03s**
Single step	13h 14m 50s	5h 12m 12s	**2h 56m 39s**
Total	52h 59m 20s	20h 37m 34s	**11h 36m 56s**

[a] DZ basis set. The ground-state geometry was used for the initial guess. HP DS25 workstation is used. [b] The first released version of the SAC-CI code. [c] With frozen-core approximation and the new back-transformation routines. CP-MOD linear equation routines were moved to link 1111. [d] Other improvements in link 1111.

4. Use of Real*4 array

The cpu memory size is important for large-scale SAC-CI calculations. All the SAC-CI results with real*4 array for ERI are almost identical to those with real*8 array as shown in table Ap-I-4 except for test640.com. We also checked this point with additional examples.

By compiling the Gaussian with activating the preprocessor flag –DUSE_R4, the SAC-CI part of the program can reduce much the cpu memory size.

Table Ap-I-4. Excitation energy for free-base porphin (test637, in eV).

State	Real*4	Real*8
$1B_{1u}$	1.767464	1.767465
$2B_{1u}$	3.575369	3.575369
$3B_{1u}$	4.141650	4.141650
$4B_{1u}$	4.922804	4.922804
$1B_{2u}$	2.246974	2.246974
$2B_{2u}$	3.705885	3.705885
$1B_{3u}$	4.329687	4.329687
$2B_{3u}$	4.854296	4.854296
$3B_{3u}$	4.422846	4.422845

5. Sorting the SAC-CI solutions in the increasing energy in the output

We changed the diagonalization routines so that the SAC-CI solutions are saved in the increasing order of energy. This is effective for the geometry optimization. According to this change, the printing order of the excited states has changed in the output.

END OF GUIDE FOR SAC-CI/Gaussian