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
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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.

4. Neutral doublet radical, for example, is calculated by the SAC-CI method as a cationic state of closed-shell anion or as an anion state of closed-shell cation. (See ref. D-6)
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. Hyperfine splitting constants of open-shell molecules.
9. 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.

I-B. References

a) Review articles


(8) H. Nakatsuji, in Computational Chemistry - Reviews of Current Trends, Vol. 2, ed. J. Leszczynski, World Scientific, 1997. For general purpose, review (8) is recommended, and for catalysis, review (7) is recommended. Biological applications are found in ref. d-20 below.

b) Related programs

(1) H. Nakatsuji, Program system for SAC and SAC-CI calculations for ground, excited, ionized, and electron-attached states. Program Library No.146 (Y4/SAC), Data Processing Center of Kyoto University, 1985. (SAC85)


(4) H. Nakatsuji, M. Hada, M. Ehara, J. Hasegawa, T. Nakajima, H. Nakai, O. Kitao, and K. Toyota, SAC/SAC-CI program system (SAC-CI96) for calculating ground, excited, ionized, and electron-attached states having singlet to septet spin multiplicities, 1996. (Delivered at the
c) Theoretical references

SAC method

SAC-CI method

SAC-CI general-\(R\) method for multi-electron excitations

SAC-CI method for high-spin states

MR-SAC and EGWF/EX-EGWF method

SAC/SAC-CI SD-\(R\) gradient method

SAC-CI general-\(R\) gradient method

MOD and MOD gradient method

d) Computational references

General

e) Integral evaluation

Integrals between configurations are evaluated using the projective reduction formalism for bonded functions developed by Reeves and others,
(1) C. M. Reeves, Comm. ACM, 9, 276 (1966).
(4) M. Hada and H. Nakatsuji, to be published. The subroutine #Projr# was modified from Projr due to B. R. Gilson.

f) Perturbation selection

Perturbation selection techniques in SAC and SAC-CI methods are explained in
(3) K. Toyota and H. Nakatsuji, submitted.

g) Eigenvalue problem of large matrices

Symmetric
Non-Symmetric

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,

\[ \psi_g = \exp(\sum_i C_i S_i) |0\rangle = (1 + \sum_i C_i S_i + \frac{1}{2} \sum_{i,j} C_i C_j S_i S_j + \ldots) |0\rangle \]
where $|0\rangle$ 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, $S^a_i$
- double excitation, $S^a_i S^b_j$

where

$$S^a_i = 1/\sqrt{2}(a^\dagger_{i\alpha} a_{i\alpha} + a^\dagger_{i\beta} a_{i\beta})$$

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

- quadruple excitation, $S(2) S(2) : S^a_i S^b_j S^c_k S^d_I$

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,

$$|\Psi_e\rangle = \sum_K d_K |\Phi_K\rangle = (\sum_K d_K R_K + \sum_K d_K C_I R_K S_I + \ldots) |0\rangle - \sum_K d_K S_{gK} |\Psi_g\rangle$$

where

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

(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

<table>
<thead>
<tr>
<th>Single</th>
<th>Double</th>
</tr>
</thead>
<tbody>
<tr>
<td>Singlet excitation</td>
<td>$S_i^a$</td>
</tr>
<tr>
<td>Triplet excitation</td>
<td>$T_i^a$</td>
</tr>
<tr>
<td>Ionization (doublet)</td>
<td>$I_i$</td>
</tr>
<tr>
<td>Electron attachment (doublet)</td>
<td>$A^a$</td>
</tr>
</tbody>
</table>

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

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

- **Single** $R_K$ * double $S_I = $ triple excitation
- **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

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>$R_{ij}^a$</th>
<th>$R_{ij}^a S_k^b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartet</td>
<td>$R_{ij}^a$</td>
<td>$R_{ij}^a S_k^b$</td>
</tr>
<tr>
<td>Quintet</td>
<td>$R_{ij}^{ab}$</td>
<td>$R_{ij}^{ab} S_{kl}$</td>
</tr>
<tr>
<td>Sextet</td>
<td>$R_{ij}^{ab}$</td>
<td>$R_{ij}^{ab} S_{lc}$</td>
</tr>
<tr>
<td>Septet</td>
<td>$R_{ijk}^{abc}$</td>
<td>$R_{ijk}^{abc} S_{ld}$</td>
</tr>
</tbody>
</table>

$R_{ij}^a = a_{aa}^\dagger a_{i\beta} a_{j\beta}$, $R_{ij}^{ab} = a_{aa}^\dagger a_{ba}^\dagger a_{i\beta} a_{j\beta}$, 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
I-C-3. Technical details - Selections of linked and unlinked operators

(A) SAC

The SAC wave function is given by

$$|\Psi_g\rangle = (1 + \sum C_i S_i + \frac{1}{2} \sum C_i C_j S_i S_j + ...) |0\rangle$$

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 $\lambda_k$, i.e.,

$$|E_s| \geq \lambda_k$$

where

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

with

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

(c) In Keyword Input

For SAC, $\lambda_k$ is automatically set by the keywords 'LevelOne/LevelTwo/LevelThree'.

Default value is $1.0 \times 10^{-3}$ (LevelThree) and others are $5.0 \times 10^{-6}$ (LevelTwo) and $1.0 \times 10^{-5}$ (LevelOne). This threshold can be input with 'EThreS2'.

2) Selection of unlinked term, $C_i C_j S_i S_j |0\rangle$

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

$$C \geq \tau_k.$$ 

Default value of $\tau_k$ is $5.0 \times 10^{-3}$. This threshold can be input with 'CThreULS2G'.

(B) SAC-CI
The SAC-CI wave function is written as
\[
|\Psi_e\rangle = \left( \sum_k d_K R_K + \sum_{k,l} d_K C_l R_K S_l + \ldots \right) |0\rangle - \sum_k d_K S_{ek} |\Psi_g\rangle.
\]

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
\[
\psi(p) = \sum_i c_i(p) \varphi_i(p) \quad (p=1,\ldots,N)
\]
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 \(\psi_s\) and define
\[
E_s(p) = \frac{|H_s(p)|^2}{E(p) - H_{ss}}
\]
where
\[
H_s(p) = \langle \psi_s | H | \psi_s \rangle, \quad E(p) = \langle \psi(p) | H | \psi(p) \rangle, \quad H_{ss} = \langle \psi_s | H | \psi_s \rangle.
\]

Now, in the selection, we include only such \(\psi_s\) which satisfies
\[
|E_s(p)| \geq \lambda_e,
\]
with at least one of the reference states \(\psi(p)\). Default value of \(\lambda_e\) for SAC-CI is given by
\[
\lambda_e = 1.0 \times 10^{-7} \quad \text{(Level Three)} \quad \text{and by} \quad 5.0 \times 10^{-7} \quad \text{(Level Two)} \quad \text{and} \quad 1.0 \times 10^{-6} \quad \text{(Level One)}.
\]
\(\lambda_e\) 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'),
\[ E_{ss}(p) = \frac{|H_{ss}(p)|^2}{(H_{ii}(p) - H_{ss})} \]

where

\[ H_{si}(p) = \langle \psi_s | H | \phi_i(p) \rangle, \quad H_{ii}(p) = \langle \phi_i(p) | H | \phi_i(p) \rangle, \quad H_{ss}(p) = \langle \psi_s | H | \psi_s \rangle. \]

Then, we include only such \( \psi_s \) which satisfies

\[ |E_{si}(p)| \geq \lambda_c.\]

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

We include only such \( \psi_s \) which satisfies

\[ |c_i(p)|^2 |E_{si}(p)| \geq \lambda'_c\]

which takes the weight of the main reference configuration into account and the default of \( \lambda'_c \) is

\[ \lambda'_c = 0.1 \times c_i(p)^2 \lambda_k.\]

2) Selection of unlinked terms,

In the unlinked term, \( \sum I d_K C_J R_K S_I \), 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 \( \tau_e \) is 0.05. These values can be input by 'CThreULS2E', 'CThreULR1' and 'CThreULR2'.

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) 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, noncanonical MOs, integral transformation)
L923 (perturbation selection, SAC/SAC-CI wavefunction, energy, and Z-vector)

if geometry optimization
L111 (2-PDM and post-SCF derivatives (including SAC/SAC-CI))
L1002 (CPHF and noncanonical MO derivatives)
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 (MOD method, reordering MOs, noncanonical MOs, integral transformation)
L923 (perturbation selection, SAC/SAC-CI wavefunction, energy)
L601 (population and related analysis)
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>
<thead>
<tr>
<th>Step</th>
<th>Job</th>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
</table>
| guide | explanations of  
1. SAC/SAC-CI program  
2. keyword input  
3. manual and namelist input  
4. input example  
5. file numbers and contents | 1. keywords for calculation | 1. stream of calculation |
| sacci1 | 1. control job stream of SAC/ SAC-CI calculation  
2. save information about the stream of calculations | 1. molecular integrals | 1. sorted molecular integrals with symmetry |
| bpres | 1. sort MO repulsion integrals from L802 or L804  
2. symmetry specification | 1. molecular integrals | 1. labels of linked operators  
2. linked operators after selection  
3. initial vectors for iterative diagonalization |
| 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. H-matrix  
2. S-matrix  
1. ci eigenvalues and eigenvectors |
| 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 |
<table>
<thead>
<tr>
<th>ulintg</th>
<th>1. integrals for unlinked terms in the SAC calculation</th>
<th>1. molecular integrals</th>
<th>1. unlinked integrals for SAC calculation</th>
</tr>
</thead>
<tbody>
<tr>
<td>sac</td>
<td>1. solve SAC non-variational equation (SAC-NV) by iterative procedure</td>
<td>1. H,S-matrix</td>
<td>1. SAC solution</td>
</tr>
<tr>
<td>dsac</td>
<td>1. solve SAC non-variational equation (SAC-NV) by iterative procedure</td>
<td>1. H,S-matrix</td>
<td>1. SAC solution</td>
</tr>
<tr>
<td>ultnt</td>
<td>1. integrals for unlinked terms in singlet SAC-CI calculations</td>
<td>1. molecular integrals</td>
<td>1. SAC-CI unlinked integrals</td>
</tr>
<tr>
<td>ultnta</td>
<td>1. integrals for unlinked terms in triplet SAC-CI calculations</td>
<td>1. molecular integrals</td>
<td>1. SAC-CI unlinked integrals</td>
</tr>
<tr>
<td>sciv</td>
<td>1. iterative SAC-CI-V solution --approximate variational—</td>
<td>1. H,S-matrix</td>
<td>1. SAC-CI-V eigenvalues and eigenvectors</td>
</tr>
<tr>
<td>das</td>
<td>1. direct SAC-CI-V solution --approximate variational—</td>
<td>1. H,S-matrix</td>
<td>1. SAC-CI-V eigenvalues and eigenvectors</td>
</tr>
<tr>
<td>scinv</td>
<td>1. iterative SAC-CI-NV solution --non-variational—</td>
<td>1. H,S-matrix</td>
<td>1. SAC-CI-NV eigenvalues and eigenvectors</td>
</tr>
<tr>
<td>dns</td>
<td>1. direct SAC-CI-NV solution --non-variational—</td>
<td>1. H,S-matrix</td>
<td>1. SAC-CI-NV eigenvalues and eigenvectors</td>
</tr>
<tr>
<td>dens</td>
<td>1. density matrices and natural orbitals for SAC and SAC-CI wave functions</td>
<td>1. SAC/SAC-CI solutions</td>
<td>1. natural orbitals</td>
</tr>
<tr>
<td></td>
<td>2. transition densities between SAC and SAC-CI wave functions</td>
<td></td>
<td>2. transition densities</td>
</tr>
<tr>
<td></td>
<td>3. spin density matrices</td>
<td></td>
<td>3. spin density matrices</td>
</tr>
<tr>
<td>prop</td>
<td>1. one-electron properties</td>
<td>1. density</td>
<td>1. one-electron properties</td>
</tr>
<tr>
<td></td>
<td>2. transition properties</td>
<td>2. natural orbital</td>
<td>2. transition properties</td>
</tr>
<tr>
<td></td>
<td>3. hyperfine splitting constant</td>
<td>3. spin density matrix</td>
<td>3. hyperfine splitting constant</td>
</tr>
</tbody>
</table>

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

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

<table>
<thead>
<tr>
<th>Step</th>
<th>Job</th>
</tr>
</thead>
<tbody>
<tr>
<td>fock</td>
<td>1. fock matrix for non-canonical orbitals</td>
</tr>
<tr>
<td>gsum</td>
<td>1. group sum of linked operators for different geometries.</td>
</tr>
<tr>
<td></td>
<td>This step is useful for calculating smooth potential surface and analytical energy gradients.</td>
</tr>
<tr>
<td>satei</td>
<td>1. intensity of ionization spectrum including shake-up process</td>
</tr>
<tr>
<td>iopc</td>
<td>1. transform MyIOp into SAC-CI one (namelist input)</td>
</tr>
<tr>
<td>fio</td>
<td>1. file I/O interface</td>
</tr>
<tr>
<td>sacutil</td>
<td>1. common subroutines used for integrals and SAC/SAC-CI analytical energy</td>
</tr>
</tbody>
</table>
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

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:

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 (CThreEgABAOp=(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 (\( \text{thrma1, thrma2, thmma1, thmma2} \)). These parameters may be different for different ISYM and KSTATE, \( \text{thrma1(ISYM,KSTATE)} \), 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 (\( \text{ETHreEgR or eseleg} \)). 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.


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

| 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 | 1 SAC and SAC-CI wave function | 1 natural orbitals |
| | 2 transition density between SAC and SAC-CI or between SAC-CI states | 2 transition density | 3 spin density matrix |
| | 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-\( \mathcal{R} \) 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-\( \mathcal{R} \)

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-\( \mathcal{R} \)
  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-\( \mathcal{R} \), 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;
  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 adapted 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 MOs 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.

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) Practically SAC/SAC-CI energy are not invariant to orbital rotations within occupied and unoccupied subspaces of MOs, due to the perturbation selection and neglect of near-zero matrix elements. Additional tasks are required to allow for this breakdown of the invariance. 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.

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).
(b) If MOD method is employed, the simultaneous linear equations derived from differentiating the corresponding conditions (see D-8) are solved.

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
   | |
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

\[ \psi_i = \sum_{\mu} \chi_\mu C_{\mu i} . \]  

(D-8:1)

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

\[ T_{ij} = U_{ij} - U_{ji} = 0 . \]  

(D-8:2)

The matrix \( U^x \) comprising so-called CPHF coefficients satisfies

\[ U^x = C^T S \frac{dC}{dx} , \]  

or equivalently

\[ \frac{dC}{dx} = CU^x . \]  

(D-8:3)

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

\[ \langle \psi_i | \frac{d}{dx} | \psi_j \rangle = 0 , \]  

(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

\[ 0x0C = MC + SC , \]  

(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

\[ M^{x_0} = 1 + (x - x_0)U^x . \]  

(D-8:6)

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

\[ 0 = T^x = U^x - (U^x)^T = (x - x_0)^{-1}(M^{x_0} - (M^{x_0})^T) . \]  

(D-8:7)
Hence
\[
(M^0 - (M^0)^T) = 0. \tag{D-8:8}
\]
The subset of MOs \( \psi_j \) satisfying Eq.(D-8:8) is obtained by the orthogonal transformations of canonical MOs \( \{ \tilde{\psi}_j \} \) as
\[
\psi_j = \sum_i \tilde{\psi}_j W_{ij}^{x_0}, \tag{D-8:9}
\]
where the transformation \( W^{x_0} \) leading to minimum orbital-deformation (MOD) is given by
\[
W^{x_0} = \left\{ (\tilde{M}^{x_0})^T \tilde{M}^{x_0} \right\}^{-1/2} (\tilde{M}^{x_0})^T, \tag{D-8:10}
\]
and
\[
\tilde{M}^{x_0} = (C^{x_0})^T S^{x_0} \tilde{C}, \tag{D-8:11}
\]
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 $C_s$ subgroups, respectively, and the corresponding tables are as follows:

<table>
<thead>
<tr>
<th>$T_d$</th>
<th>$D_2$</th>
<th>$C_{3v}$</th>
<th>$C_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>A</td>
<td>A1</td>
<td>A'</td>
</tr>
<tr>
<td>A2</td>
<td>A</td>
<td>A2</td>
<td>A''</td>
</tr>
<tr>
<td>E</td>
<td>A</td>
<td>E</td>
<td>A',A''</td>
</tr>
<tr>
<td>T1</td>
<td>B1,B2,B3</td>
<td>T1</td>
<td>B1,B2,B3</td>
</tr>
<tr>
<td>T2</td>
<td>B1,B2,B3</td>
<td>T2</td>
<td>B1,B2,B3</td>
</tr>
</tbody>
</table>

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 $T_d$, 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 $A_1$ and $A_2$ in $C^*_2$) is not necessary. In calculating the $E$ state of $T_d$, $(A,B_1,B_2,B_3)=(2,0,0,0)$ 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 unoccupied (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 $\text{Sqrt}(3.0)$. 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 CH₄. 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) Cₙ groups

<table>
<thead>
<tr>
<th>C₃ → C₁</th>
<th>C₄ → C₂</th>
<th>C₅ → C₁</th>
<th>C₆ → C₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>A → A</td>
<td>A → A</td>
<td>A → A</td>
<td>A → A</td>
</tr>
<tr>
<td>E → 2A</td>
<td>B → A</td>
<td>E₁ → 2A</td>
<td>B → B</td>
</tr>
<tr>
<td>E → 2B</td>
<td>E₂ → 2A</td>
<td>E₁ → 2B</td>
<td>E₂ → 2A</td>
</tr>
</tbody>
</table>

(2) Cₙᵥ groups

<table>
<thead>
<tr>
<th>C₃ᵥ → C₄</th>
<th>C₄ᵥ → C₂ᵥ</th>
<th>C₅ᵥ → C₄</th>
<th>C₆ᵥ → C₂ᵥ</th>
<th>C₅ᵥ → C₂ᵥ</th>
</tr>
</thead>
<tbody>
<tr>
<td>A₁ → A’</td>
<td>A₁ → A₁</td>
<td>A₁ → A’</td>
<td>A₁ → A₁</td>
<td>σ⁺ → A₁</td>
</tr>
<tr>
<td>A₂ → A”</td>
<td>A₂ → A₂</td>
<td>A₂ → A”</td>
<td>A₂ → A₂</td>
<td>σ⁻ → A₂</td>
</tr>
<tr>
<td>E → A’+A”</td>
<td>(B₁,B₂) → (A₁,A₂)</td>
<td>E₁ → 2B</td>
<td>(B₁,B₂) → (B₁,B₂)</td>
<td>Π → B₁+B₂</td>
</tr>
<tr>
<td>E → B₁+B₂</td>
<td>E₂ → 2A</td>
<td>E₁ → B₁+B₂</td>
<td>Δ → A₁+A₂</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>E₂ → A₁+A₂</td>
<td></td>
<td>---</td>
</tr>
</tbody>
</table>

(3) Cₙₕ groups

<table>
<thead>
<tr>
<th>C₃ₕ → C₅</th>
<th>C₄ₕ → C₂ₕ</th>
<th>C₅ₕ → C₃</th>
<th>C₆ₕ → C₂ₕ</th>
</tr>
</thead>
<tbody>
<tr>
<td>A’ → A’</td>
<td>A₉ → A₉</td>
<td>A’ → A’</td>
<td>A₉ → A₉</td>
</tr>
<tr>
<td>E’ → 2A’</td>
<td>B₉ → A₉</td>
<td>E₁’ → 2A’</td>
<td>B₉ → B₉</td>
</tr>
<tr>
<td>A” → A”</td>
<td>E₉ → 2B₉</td>
<td>E₂’ → 2A’</td>
<td>E₁₉ → 2B₉</td>
</tr>
<tr>
<td>E” → 2A”</td>
<td>Aₙ → Aₙ</td>
<td>A” → A”</td>
<td>E₂₉ → 2A₉</td>
</tr>
<tr>
<td></td>
<td>Bₙ → Aₙ</td>
<td>E₁” → 2A”</td>
<td>Aₙ → Aₙ</td>
</tr>
<tr>
<td></td>
<td>Eₙ → 2Bₙ</td>
<td>E₂” → 2A”</td>
<td>Bₙ → Bₙ</td>
</tr>
<tr>
<td></td>
<td>E₁u → 2Bₘ</td>
<td></td>
<td>E₁u → 2Bₘ</td>
</tr>
<tr>
<td></td>
<td>E₂u → 2Aₘ</td>
<td></td>
<td>E₂u → 2Aₘ</td>
</tr>
</tbody>
</table>

27
### (4) $D_n$ groups

<table>
<thead>
<tr>
<th>$D_3 \to C_2$</th>
<th>$D_4 \to D_2$</th>
<th>$D_5 \to C_2$</th>
<th>$D_6 \to D_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1 \to A$</td>
<td>$A_1 \to A$</td>
<td>$A_1 \to A$</td>
<td>$A_1 \to A$</td>
</tr>
<tr>
<td>$A_2 \to B$</td>
<td>$A_2 \to B_1$</td>
<td>$A_2 \to B$</td>
<td>$A_2 \to B_1$</td>
</tr>
<tr>
<td>$E \to A+B$</td>
<td>$(B_1,B_2) \to (A,B_1)$</td>
<td>$E_1 \to A + B$</td>
<td>$(B_1,B_2) \to (B_2,B_3)$</td>
</tr>
<tr>
<td></td>
<td>$E_1 \to B_2+B_3$</td>
<td>$E_2 \to A + B$</td>
<td>$E_1 \to B_2+B_3$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$E_2 \to A + B$</td>
<td></td>
</tr>
</tbody>
</table>

### (5) $D_{nd}$ groups

<table>
<thead>
<tr>
<th>$D_{2d} \to C_{2v}$</th>
<th>$D_{3d} \to C_{2h}$</th>
<th>$D_{4d} \to C_{2v}$</th>
<th>$D_{5d} \to C_{2h}$</th>
<th>$D_{6d} \to C_{2v}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1 \to A_1$</td>
<td>$A_{1g} \to A_g$</td>
<td>$A_1 \to A_1$</td>
<td>$A_{1g} \to A_g$</td>
<td>$A_1 \to A_1$</td>
</tr>
<tr>
<td>$A_2 \to A_2$</td>
<td>$A_{2g} \to B_g$</td>
<td>$A_2 \to A_2$</td>
<td>$A_{2g} \to B_g$</td>
<td>$A_2 \to A_2$</td>
</tr>
<tr>
<td>$B_1 \to A_2$</td>
<td>$E_g \to A_g + B_g$</td>
<td>$B_1 \to A_2$</td>
<td>$E_{1g} \to A_g + B_g$</td>
<td>$B_1 \to A_2$</td>
</tr>
<tr>
<td>$B_2 \to A_1$</td>
<td>$A_{1u} \to A_u$</td>
<td>$B_2 \to A_1$</td>
<td>$E_{2g} \to A_g + B_g$</td>
<td>$B_2 \to A_1$</td>
</tr>
<tr>
<td>$E \to B_1 + B_2$</td>
<td>$A_{2u} \to B_u$</td>
<td>$E_1 \to B_1 + B_2$</td>
<td>$A_{1u} \to A_u$</td>
<td>$E_1 \to B_1 + B_2$</td>
</tr>
<tr>
<td></td>
<td>$E_u \to A_u + B_u$</td>
<td>$E_2 \to A_1 + A_2$</td>
<td>$A_{2u} \to B_u$</td>
<td>$E_2 \to A_1 + A_2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$E_3 \to B_1 + B_2$</td>
<td>$E_{1u} \to A_u + B_u$</td>
<td>$E_3 \to B_1 + B_2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$E_{2u} \to A_u + B_u$</td>
<td>$E_4 \to A_1 + A_2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$E_5 \to B_1 + B_2$</td>
</tr>
</tbody>
</table>

### (6) $D_{nh}$ groups

<table>
<thead>
<tr>
<th>$D_{3h} \to C_{2v}$</th>
<th>$D_{4h} \to D_{2h}$</th>
<th>$D_{5h} \to C_{2v}$</th>
<th>$D_{6h} \to D_{2h}$</th>
<th>$D_{nh} \to D_{2h}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1' \to A_1$</td>
<td>$A_{1g} \to A_g$</td>
<td>$A_1' \to A_1$</td>
<td>$A_{1g} \to A_g$</td>
<td>$\Sigma^+ \to A_g$</td>
</tr>
<tr>
<td>$A_2' \to B_1$</td>
<td>$A_{2g} \to B_{1g}$</td>
<td>$A_2' \to B_1$</td>
<td>$A_{2g} \to B_{1g}$</td>
<td>$\Sigma^- \to B_{1g}$</td>
</tr>
<tr>
<td>$E' \to A_1 + B_1$</td>
<td>$(B_{1g},B_{2g}) \to (A_{g_1},B_{1g})$</td>
<td>$E_1' \to A_1 + B_1$</td>
<td>$(B_{1g},B_{2g}) \to (B_{1g},B_{3g})$</td>
<td>$\Pi \to B_{2g} + B_{3g}$</td>
</tr>
<tr>
<td>$A_{1''} \to A_2$</td>
<td>$E_g \to B_{2g} + B_{3g}$</td>
<td>$E_2' \to A_1 + B_1$</td>
<td>$E_{1g} \to B_{2g} + B_{3g}$</td>
<td>$\Delta \to A_g + B_{1g}$</td>
</tr>
<tr>
<td>$A_2'' \to B_2$</td>
<td>$A_{1u} \to A_u$</td>
<td>$A_{1''} \to A_2$</td>
<td>$E_{2g} \to A_g + B_{1g}$</td>
<td>---</td>
</tr>
<tr>
<td>$E'' \to A_2 + B_2$</td>
<td>$A_{2u} \to B_{1u}$</td>
<td>$E_{1''} \to A_2 + B_2$</td>
<td>$A_{1u} \to A_u$</td>
<td>$\Sigma^+ \to B_{1u}$</td>
</tr>
<tr>
<td></td>
<td>$(B_{1u},B_{2u}) \to (A_{u_1},B_{1u})$</td>
<td>$E_{1''} \to A_2 + B_2$</td>
<td>$A_{2u} \to B_{1u}$</td>
<td>$\Sigma^- \to A_u$</td>
</tr>
<tr>
<td></td>
<td>$E_u \to B_{2u} + B_{3u}$</td>
<td>$E_{2''} \to A_2 + B_2$</td>
<td>$(B_{1u},B_{2u}) \to (B_{2u},B_{3u})$</td>
<td>$\Pi \to B_{2u} + B_{3u}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$E_{1u} \to B_{2u} + B_{3u}$</td>
<td>$\Delta \to A_u + B_{1u}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$E_{2u} \to A_u + B_{1u}$</td>
<td>---</td>
</tr>
</tbody>
</table>

### (7) $S_n$ groups

<table>
<thead>
<tr>
<th>$S_4 \to C_2$</th>
<th>$S_6 \to C_1$</th>
<th>$S_8 \to C_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A \to A$</td>
<td>$A_g \to A_g$</td>
<td>$A \to A$</td>
</tr>
<tr>
<td>$B \to A$</td>
<td>$E_g \to 2A_g$</td>
<td>$B \to A$</td>
</tr>
<tr>
<td>$E \to 2B$</td>
<td>$A_u \to A_u$</td>
<td>$E_1 \to 2B$</td>
</tr>
</tbody>
</table>
(8) Polyhedral groups

| Group | Td | O
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>A₁ → A</td>
<td>A₁g → A₁g</td>
<td>A₁g → A₁g</td>
</tr>
<tr>
<td>A₂ → A</td>
<td>A₂g → A₁g</td>
<td>A₂g → A₁g</td>
</tr>
<tr>
<td>E → 2A</td>
<td>E₁g → 2A₁g</td>
<td>E₁g → 2A₁g</td>
</tr>
<tr>
<td>T₁ → B₁ + B₂ + B₃</td>
<td>T₁g → B₁g + B₂g + B₃g</td>
<td>T₁u → B₁u + B₂u + B₃u</td>
</tr>
<tr>
<td>T₂ → B₁ + B₂ + B₃</td>
<td>T₂g → B₁g + B₂g + B₃g</td>
<td>T₂u → B₁u + B₂u + B₃u</td>
</tr>
<tr>
<td>E₁u → A₁u</td>
<td>A₁u → A₁u</td>
<td></td>
</tr>
<tr>
<td>A₂u → A₂u</td>
<td>A₂u → A₂u</td>
<td></td>
</tr>
<tr>
<td>E₁u → 2A₁u</td>
<td>E₁u → 2A₁u</td>
<td></td>
</tr>
<tr>
<td>T₁u → B₁u + B₂u + B₃u</td>
<td>T₁u → B₁u + B₂u + B₃u</td>
<td></td>
</tr>
<tr>
<td>T₂u → B₁u + B₂u + B₃u</td>
<td>T₂u → B₁u + B₂u + B₃u</td>
<td></td>
</tr>
</tbody>
</table>

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 algorithms can be used. The direct algorithm recalculates AO integrals when they are required. The conventional algorithm uses AO integrals which are already stored on disk. We recommend the direct algorithm and this is the default.

Within the direct transformation, the in-core, fully-direct, and semi-direct algorithms are available. In the default, the program will select the best algorithm 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 \( N^*(N-1)/4/N_{rep} \) words, where \( N=N_{act}*(N_{act}-1)/2 \), \( N_{act} \) is the active space of SAC/SAC-CI and \( N_{rep} \) 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 exceed the disk space, job terminates. In large-scale calculations where the size of RWF may exceed 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*

<table>
<thead>
<tr>
<th>State</th>
<th>SAC-CI-NV</th>
<th>EOM-CC</th>
<th>Full-CI</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Full</td>
<td>#1</td>
<td>#2</td>
</tr>
<tr>
<td>Singlet</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
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.

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.

<table>
<thead>
<tr>
<th>parameter</th>
<th>variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>#01</td>
<td>Number of primitive gaussians at scf level. #prop#</td>
</tr>
<tr>
<td>#02</td>
<td>Number of ao's.</td>
</tr>
<tr>
<td>#03</td>
<td>Number of mo's. #eri#</td>
</tr>
<tr>
<td>#04</td>
<td>Number of active mo's used in moeri calculation.</td>
</tr>
<tr>
<td>#05</td>
<td>SD-CI dimension after perturbation selection (should be larger than #06).</td>
</tr>
<tr>
<td>#06</td>
<td>Unit for i/o transfer (should be larger than the dimension #14 at #das#, #dsac# and #dnas#).</td>
</tr>
<tr>
<td>#07</td>
<td>Number of solutions + maximum number of iterations before &quot;refresh&quot; in #cid#, #sciv#, and #scinv#.</td>
</tr>
<tr>
<td>#08</td>
<td>SE-CI dimension without symmetry.</td>
</tr>
<tr>
<td>#09</td>
<td>SE-CI dimension with symmetry.</td>
</tr>
<tr>
<td>#10</td>
<td>DE-CI dimension without symmetry before perturbation selection.</td>
</tr>
<tr>
<td>#11</td>
<td>DE-CI dimension with symmetry before perturbation selection.</td>
</tr>
<tr>
<td>#12</td>
<td>DE-CI dimension with symmetry after perturbation selection.</td>
</tr>
<tr>
<td>#13</td>
<td>= 2, when kblock='kblock' as ordinary is.</td>
</tr>
<tr>
<td></td>
<td>= 3, when kblock='double', namely when doubly excited configurations are used as main reference configuration in perturbation selection step.</td>
</tr>
<tr>
<td>#14</td>
<td>Dimension in direct diagonalization steps, #dsac#, #das#, and #dnas#.</td>
</tr>
<tr>
<td>#15</td>
<td>Maximum number of solutions in direct diagonalization steps, #das# and #dnas#.</td>
</tr>
<tr>
<td>#16</td>
<td>Array for integral sorting in #isort#.</td>
</tr>
<tr>
<td>#17</td>
<td>Number of transformed 2-electron repulsion integrals (only symmetrically non-zero integrals are stored.).</td>
</tr>
<tr>
<td>#18</td>
<td>Number of configurations (before selection) taken into perturbation selection subroutine.</td>
</tr>
</tbody>
</table>

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

\[
\begin{align*}
NAT(2) &= #01 \\
NAT(4) &= #02 \\
NAT(6) &= NAT(4) \times NAT(4) \\
NAT(8) &= (NAT(4)+1) \times NAT(4)/2 \\
NAT(10) &= NAT(4) \times 7 \\
NAT(12) &= NAT(8)+3 \\
NAT(14) &= NAT(4) \times NAT(8)
\end{align*}
\]
\begin{align*}
\text{NAT}(16) &= 03 \\
\text{NAT}(18) &= (\text{NAT}(16)+1)*\text{NAT}(16)/2 \\
\text{NAT}(20) &= \text{int}(\text{NAT}(16)/2) \\
\text{NAT}(22) &= 04 \\
\text{NAT}(24) &= \text{NAT}(26)*(\text{NAT}(26)+1)/2 \\
\text{NAT}(26) &= \text{NAT}(22)*(\text{NAT}(22)+1)/2 \\
\text{NAT}(28) &= \text{NAT}(22)*7 \\
\text{NAT}(30) &= 05 \text{ (should be larger than NAT}(32)) \\
\text{NAT}(32) &= 06 \text{ (should be larger than NAT}(60)) \\
\text{NAT}(34) &= 07 \\
\text{NAT}(36) &= \text{NAT}(34)*(\text{NAT}(34)+1)/2 \\
\text{NAT}(38) &= \text{NAT}(34)+1 \\
\text{NAT}(40) &= \text{NAT}(34)+3 \\
\text{NAT}(41) &= \text{NAT}(34)*2 \\
\text{NAT}(42) &= 08 \\
\text{NAT}(44) &= 09 \\
\text{NAT}(46) &= (\text{NAT}(44)+1)*\text{NAT}(44)/2 \\
\text{NAT}(48) &= \text{NAT}(44)*7 \\
\text{NAT}(50) &= 10 \\
\text{NAT}(52) &= 11 \\
\text{NAT}(54) &= 12 \text{ (will be modified in pres-cimx)} \\
\text{NAT}(56) &= 13 \\
\text{NAT}(58) &= \text{NAT}(32) \\
\text{NAT}(60) &= 14 \\
\text{NAT}(62) &= \text{NAT}(60)*(\text{NAT}(60)+1)/2 \\
\text{NAT}(63) &= \text{NAT}(60)*2 \text{ (numpac)} \\
\text{NAT}(64) &= \text{NAT}(60)*5 \text{ (facom)} \\
\text{NAT}(65) &= \text{NAT}(60)+1 \text{ (numpac)} \\
\text{NAT}(66) &= \text{NAT}(60)*6 \text{ (numpac)} \\
\text{NAT}(68) &= 15 \\
\text{NAT}(70) &= 16 \\
\text{NAT}(99) &= 17
\end{align*}

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

$$|\Psi^{\text{SAC}}\rangle = \exp \left( \sum_{i=1}^{M} C_i S_i \right) |\Phi_0\rangle,$$

with a closed-shell determinant $|\Phi_0\rangle$, which is usually Hartree-Fock, and the SAC-CI wave functions are expressed using the SAC wave function as

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

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.

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.

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 \( \text{MaxR} \leq 6 \). 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 \( \text{MaxR} \leq 4 \) and then to perform perturbation selection as above. (\text{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**

\[ \text{NState} = (N1,...,N8) \]

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. 
\( \text{NState} = N \) means \( \text{NState} = (N,N,\ldots) \).

# 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 \( \text{NState} = (N1,N2,N3,N4) \).
# For degenerate symmetry, the SAC-CI calculation is done in a closest linear symmetry (\( D_2 \) for Td, for example) and \( \text{NState} \) option is given for this linear symmetry (\( \text{NState}=(1,2,0,0) \) 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 SelectCISonly.)

Max\( R = N \) sets the maximum excitation level, \( N \), (\( N \leq 6 \) for EgOp, \( N \leq 4 \) 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 general-R LevelTwo calculation of the ionized states of a molecule in D₂ symmetry with the R-operators up to quadruples within the active space of the second to 14-th MOs.

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

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) [11,12] condition to avoid singularities in the energy gradient calculations. See CPHF. When MOD is used, the active orbital space is automatically forced to be Full and not compatible with FC (FrozenCore) in the present version.

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
```

40
Calc. GSUM from R=5.0 to R=12.0 au.

\begin{verbatim}
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
\end{verbatim}

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

\begin{verbatim}
0 1
Li
Li 1 R1
R1 12.0 8 -1.0
\end{verbatim}

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

SelectCISonly 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 g01/tests/sgi.

References

(2) SAC/SAC-CI GUIDE, in the present SAC-CI homepage.

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 calculation of 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**

sets CThre for selecting A and B operators of the A*B term in the exponential generation

=(subword)

subword

A1Op = val

sets CThre for A1 operator to var.

A2Op = val

sets CThre for A2 operator to var.

**CThreEgAABAOp**

sets CThre for selecting A and B operators of the A*A*B term in the exponential generation

=(sub-description)

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 = $n$
- $n=0$: activates perturbation selection using reference states. (default)
- $n=1$: activates perturbation selection using (coefficients)**2.
- $n=2$: 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.

PlusULSACCI = (terms)
requests to add unlinked terms in SAC-CI specified by terms in addition to R1S2 and R2S2 is used in default.

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

EThreEgR = $val$
specifies energy-threshold in perturbation for higher-order general-$R$ operators.

CThreEgAB
sets CThre for selecting A and B operators of the A*B terms in the exponential generation

$(subword)$
B1Op = $val$
sets CThre for B1 operator to var.

B2Op = $val$
sets CThre for B2 operator to var.

CThreEgAAB
sets CThre for selecting A and B operators of the A*A*B terms in the exponential generation (Eg) scheme.

$(subword)$
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

\textbf{ConvLin} = M \quad \text{sets the energy convergence criterion to } 10^{\text{(-M)}} \text{ in solving the linear equation of SAC.}

\textbf{MaxItLin} = N \quad \text{sets the maximum iteration to } N \text{ in solving the linear equation of SAC.}

\textbf{Omega} = N \quad \text{sets a parameter for relaxation method in the linear equation of SAC.}

\textbf{CutoffDIIS} = \text{var} \quad \text{sets a cut-off parameter for DIIS in SAC.}

\textbf{CutoffDIISZVec} = \text{var} \quad \text{sets a cut-off parameter for DIIS in the Z-vector method.}

---

Detailed Keywords for Print Control

\#P \quad \#P \text{ requests more printing.}

\textbf{PrintOperator} \quad \text{requests to print out all excitation operators.}

\textbf{PrintNaturalOrbital} \quad \text{requests to print out the natural orbitals.}

\textbf{PrintDensityMatrix} \quad \text{requests to print out the density matrix.}

\textbf{PrintMyIOp} \quad \text{requests to print out MyIOp.}

---

Detailed Keywords for Name-List Input and Restart

\textbf{Namelist} \quad \text{forces to read namelist input.}

\textbf{Restart} \quad \text{requests to re-start from the last link.}

---

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

\begin{center}
\begin{tabular}{|l|l|l|}
\hline
Keyword & Short explanation & Default action \\
\hline
\textbf{===== STANDARD KEYWORDS =====} & & \\
\hline
\textbf{REFERENCE MO FOR SAC/SAC-CI AND INTEGRAL TRANSFORMATION} & & \\
LMO & Localized MO & Canonical \\
FullActive & Full Active Space & Gaussian’s standard \\
Window & Active Space & Gaussian’s standard \\
RefCIWindow & reference CI Window & Window \\
\hline
\textbf{SAC-CI KEYWORDS:} & & \\
\textbf{ACCURACY} & & \\
SD-\textit{R}/General-\textit{R} & \textit{R}-operators & SD-\textit{R} \\
LevelOne/LevelTwo/LevelThree & Accuracy of calculation of perturbation selection of linked operators & LevelThree \\
NoLinkedSelection & Suppress selection & LinkedSelection \\
\hline
\end{tabular}
\end{center}
FullRGGeneration Generates all higher linked operators in general-\( R \) SAC-CI

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
MaxR Maximum order of \( R \) 6 for singlet to quintet in general-\( R \) 4 for sextet to septet

GRADIENT CALCULATION AND GEOMETRY OPTIMIZATION

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

RELATED KEYWORDS

CPHF Type of derivatives MOD
Force - Gaussian's standard
Op - 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 4 for single point
10**(-N) 5 for gradient
DConvSAC=N Convergence threshold 6 for single point
10**(-N) 7 for gradient
### DENSITY AND TRANSITION DENSITY

<table>
<thead>
<tr>
<th>TransitionFrom</th>
<th>Specify initial state</th>
</tr>
</thead>
<tbody>
<tr>
<td>SpinState=spin</td>
<td>Spin-state name singlet</td>
</tr>
<tr>
<td>Symmetry=M</td>
<td>Symmetry number 1</td>
</tr>
<tr>
<td>Root=N</td>
<td>Solution number 0 (SAC state)</td>
</tr>
<tr>
<td>AllProperties</td>
<td>All property not activated</td>
</tr>
<tr>
<td>NoProperty</td>
<td>No property not activated</td>
</tr>
</tbody>
</table>

### GSUM (GROUP SUM OF SELECTED OPERATORS)

| BeforeGSUM/CalcGSUM/AfterGSUM | not activated |

### MEMORY REQUIREMENT

<table>
<thead>
<tr>
<th>MaxR2Op</th>
<th>Buffer of R2 operator 100000</th>
</tr>
</thead>
<tbody>
<tr>
<td>MaxEgOp</td>
<td>Buffer of higher- operator 10000</td>
</tr>
</tbody>
</table>

### OTHERS

| SelecCISonly | CIS and selection only not activated |

#### === DETAILED KEYWORDS ===

<table>
<thead>
<tr>
<th>SAC</th>
</tr>
</thead>
<tbody>
<tr>
<td>EThreS2</td>
</tr>
<tr>
<td>CThreMainConfig</td>
</tr>
<tr>
<td>CThreULS2G</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>SAC-CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>CThreULS2E</td>
</tr>
<tr>
<td>CThreULR1</td>
</tr>
<tr>
<td>CThreULR2</td>
</tr>
<tr>
<td>CThreDensULS2</td>
</tr>
<tr>
<td>CThreDensULR1</td>
</tr>
<tr>
<td>RefCISD</td>
</tr>
<tr>
<td>EThreDegFac</td>
</tr>
<tr>
<td>CThreDegULFac</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>GENERAL-R</th>
</tr>
</thead>
<tbody>
<tr>
<td>EgOp</td>
</tr>
<tr>
<td>CThreEgABAOp=</td>
</tr>
<tr>
<td>A1Op</td>
</tr>
<tr>
<td>A2Op</td>
</tr>
<tr>
<td>CThreEgAABAOp=</td>
</tr>
<tr>
<td>A1Op</td>
</tr>
<tr>
<td>A2Op</td>
</tr>
<tr>
<td>EgAOp=</td>
</tr>
</tbody>
</table>
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  SkipSmallCI
FullRGeneration

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 linear equation  200
CutoffDIIS  Cut-off parameter  0.01
CutoffDIISZVec  Cut-off parameter  0.1

PRINT CONTROL
#P  Extra pringing  not activated
PrintOperator  Print operators  not activated
PrintNaturalOrbital  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.

<table>
<thead>
<tr>
<th>State</th>
<th>Density (WITHHF)</th>
<th>Transition density</th>
<th>Transition density among SAC-CI states</th>
</tr>
</thead>
<tbody>
<tr>
<td>Singlet state</td>
<td>&lt;L</td>
<td>O</td>
<td>R&gt;</td>
</tr>
<tr>
<td>Other spin multiplicity</td>
<td>&lt;L</td>
<td>O</td>
<td>R&gt;</td>
</tr>
</tbody>
</table>

* <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--

Actual input and output lists are given in Part V of this manual.

### Input 631 ###  H$_2$O with DZ basis - comparison with full-CI

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$_2$O calculated by the SAC-CI and Full-CI (FCI) methods.###

<table>
<thead>
<tr>
<th>State</th>
<th>Orbital Picture$^{[a]}$</th>
<th>Method</th>
<th>Dim.</th>
<th>Total Energy (Hatree)$^{[b]}$</th>
<th>Error (mHatree)$^{[c]}$</th>
<th>$E_{ex}$ (eV)$^{[d]}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Singlet states</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>XA$_1$</td>
<td>HF det.</td>
<td>SAC</td>
<td>361</td>
<td>-76.156254</td>
<td>1.61</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FCI</td>
<td>256474</td>
<td>-76.157866</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2A$_1$</td>
<td>n $\rightarrow$ 3s</td>
<td>SAC-CI</td>
<td>361</td>
<td>-75.761035</td>
<td>-1.52</td>
<td>10.75</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FCI</td>
<td>256474</td>
<td>-75.759512</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3A$_1$</td>
<td>$\sigma$ $\rightarrow$ 3py</td>
<td>SAC-CI</td>
<td>361</td>
<td>-75.454280</td>
<td>3.30</td>
<td>19.10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FCI</td>
<td>256474</td>
<td>-75.457584</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1A$_2$</td>
<td>$\pi$ $\rightarrow$ 3py</td>
<td>SAC-CI</td>
<td>192</td>
<td>-75.457584</td>
<td>-0.92</td>
<td>10.73</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FCI</td>
<td>245000</td>
<td>-75.761966</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1B$_1$</td>
<td>$\pi$ $\rightarrow$ 3s</td>
<td>SAC-CI</td>
<td>216</td>
<td>-75.840435</td>
<td>-2.14</td>
<td>8.59</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FCI</td>
<td>245776</td>
<td>-75.838288</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1B$_2$</td>
<td>n $\rightarrow$ 3py</td>
<td>SAC-CI</td>
<td>312</td>
<td>-75.670341</td>
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<td>13.22</td>
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<td></td>
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<td>FCI</td>
<td>254752</td>
<td>-75.670141</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2B$_2$</td>
<td>$\sigma$ $\rightarrow$ 3s</td>
<td>SAC-CI</td>
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</tr>
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<td>FCI</td>
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<td></td>
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<tr>
<td>Triplet states</td>
<td></td>
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<tr>
<td>1A$_1$</td>
<td>n $\rightarrow$ 3s</td>
<td>SAC-CI</td>
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<td></td>
</tr>
<tr>
<td>2A$_1$</td>
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<tr>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>1A$_2$</td>
<td>$\pi$ $\rightarrow$ 3py</td>
<td>SAC-CI</td>
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<td>-0.34</td>
<td>10.23</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FCI</td>
<td>437640</td>
<td>-75.779926</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1B$_1$</td>
<td>$\pi$ $\rightarrow$ 3s</td>
<td>SAC-CI</td>
<td>294</td>
<td>-75.869964</td>
<td>-2.46</td>
<td>7.79</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FCI</td>
<td>437520</td>
<td>-75.867507</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1B$_2$</td>
<td>n $\rightarrow$ 3py</td>
<td>SAC-CI</td>
<td>410</td>
<td>-75.722134</td>
<td>-0.51</td>
<td>11.81</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FCI</td>
<td>441120</td>
<td>-75.721626</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2B$_2$</td>
<td>$\sigma$ $\rightarrow$ 3s</td>
<td>SAC-CI</td>
<td>410</td>
<td>-75.634992</td>
<td>0.85</td>
<td>14.18</td>
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<tr>
<td></td>
<td></td>
<td>FCI</td>
<td>441120</td>
<td>-75.635841</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ionized states</td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>1A$_1$</td>
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<td>SAC-CI</td>
<td>82</td>
<td>-75.663487</td>
<td>-7.81</td>
<td>13.41</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FCI</td>
<td>232968</td>
<td>-75.655680</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1B$_1$</td>
<td>$\pi$</td>
<td>SAC-CI</td>
<td>48</td>
<td>-75.728794</td>
<td>-8.56</td>
<td>11.63</td>
</tr>
</tbody>
</table>

---

[a] $^{[a]}$ Orbital Picture: $\sigma$ for bonding orbitals, $\pi$ for antibonding orbitals.
[b] $^{[b]}$ Total Energy in Hatrees ($\text{H}_{\text{a}}$).
[c] $^{[c]}$ Error in milli-Hatrees (m$\text{H}_{\text{a}}$).
[d] $^{[d]}$ Excitation Energy in electron-volts (eV).
Electron-attached states

1A1  3s  SAC-CI  150  -75.959222   5.36
1B1  3p_x  SAC-CI  72  -75.321567  22.71
1B2  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 ### H2O with DZ1P plus Rydberg basis

1. Singlet and triplet excited states of H2O are calculated with DZ1P plus Rydberg [2s2p] functions. The results compare well with the experimental values.

References:

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 H2O.

<table>
<thead>
<tr>
<th>State</th>
<th>Orbital picture</th>
<th>SAC-CI</th>
<th>Exptl.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>E_{ex}(eV)</td>
<td>Osc.(au)</td>
<td>E_{ex}(eV)</td>
</tr>
<tr>
<td>Singlet states</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1B_1</td>
<td>π → 3s(OH^*), π → 4s</td>
<td>7.36</td>
<td>0.0556</td>
</tr>
<tr>
<td>1A_2</td>
<td>π → 3p_y, π → 4p_y</td>
<td>9.25</td>
<td>0.0000</td>
</tr>
<tr>
<td>2A_1</td>
<td>π → 3p_x, n → 3s</td>
<td>9.71</td>
<td>0.0566</td>
</tr>
<tr>
<td>2B_1</td>
<td>π → 3p_z</td>
<td>9.83</td>
<td>0.0079</td>
</tr>
<tr>
<td>3A_1</td>
<td>π → 3p_x, n → 3s</td>
<td>10.01</td>
<td>0.0449</td>
</tr>
<tr>
<td>3B_1</td>
<td>π → 4s, π → 3s</td>
<td>11.24</td>
<td>0.0073</td>
</tr>
<tr>
<td>1B_2</td>
<td>n → 3p_y, n → 4p_y</td>
<td>11.63</td>
<td>0.0143</td>
</tr>
<tr>
<td>2A_2</td>
<td>π → 4p_y, π → 3p_y</td>
<td>11.72</td>
<td>0.0000</td>
</tr>
<tr>
<td>4B_1</td>
<td>n → 3p_z</td>
<td>12.09</td>
<td>0.0002</td>
</tr>
<tr>
<td>4A_1</td>
<td>n → 3p_z</td>
<td>12.13</td>
<td>0.0036</td>
</tr>
<tr>
<td>5A_1</td>
<td>π → 4p_x</td>
<td>12.91</td>
<td>0.0038</td>
</tr>
<tr>
<td>Triplet states</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1B_1</td>
<td>π → 3s(OH^*), π → 4s</td>
<td>6.97</td>
<td>-</td>
</tr>
<tr>
<td>1A_2</td>
<td>π → 3p_y, π → 4p_y</td>
<td>9.11</td>
<td>-</td>
</tr>
<tr>
<td>1A_1</td>
<td>n → 3s(OH^*), n → 4s</td>
<td>9.39</td>
<td>-</td>
</tr>
<tr>
<td>2A_1</td>
<td>π → 3p_x, π → 4p_x</td>
<td>9.58</td>
<td>-</td>
</tr>
<tr>
<td>2B_1</td>
<td>π → 3p_z</td>
<td>9.78</td>
<td>-</td>
</tr>
<tr>
<td>3B_1</td>
<td>π → 4s, π → 3s</td>
<td>10.98</td>
<td>-</td>
</tr>
<tr>
<td>1B_2</td>
<td>n → 3p_y, n → 4p_y</td>
<td>11.39</td>
<td>-</td>
</tr>
<tr>
<td>2A_2</td>
<td>π → 4p_y, π → 3p_y</td>
<td>11.49</td>
<td>-</td>
</tr>
<tr>
<td>3A_1</td>
<td>n → 3p_z</td>
<td>11.89</td>
<td>-</td>
</tr>
<tr>
<td>4B_1</td>
<td>n → 3p_x</td>
<td>12.04</td>
<td>-</td>
</tr>
<tr>
<td>4A_1</td>
<td>π → 4p_x</td>
<td>12.30</td>
<td>-</td>
</tr>
</tbody>
</table>
Ionized (Cation doublet) states

<table>
<thead>
<tr>
<th>State</th>
<th>Orbital picture</th>
<th>SAC-CI</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>&lt;r&gt;</td>
</tr>
<tr>
<td>1B1</td>
<td>π → 3s(OH*)</td>
<td>12.19</td>
</tr>
<tr>
<td>1A1</td>
<td>n</td>
<td>14.52</td>
</tr>
<tr>
<td>1B2</td>
<td>σ</td>
<td>18.88</td>
</tr>
</tbody>
</table>

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 H2O.

<table>
<thead>
<tr>
<th>State</th>
<th>Orbital picture</th>
<th>DM</th>
<th>Second Moment</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>&lt;r&gt;</td>
<td>&lt;x^2&gt;</td>
</tr>
<tr>
<td>Singlet states</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>XA1</td>
<td>HF det.</td>
<td>-0.87</td>
<td>5.84</td>
</tr>
<tr>
<td>1B1</td>
<td>π → 3s(OH*)</td>
<td>0.67</td>
<td>10.86</td>
</tr>
<tr>
<td></td>
<td>π → 4s</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1A2</td>
<td>π → 3p_y, π → 4p_y</td>
<td>-0.80</td>
<td>11.77</td>
</tr>
<tr>
<td>2A1</td>
<td>π → 3p_x, n → 3s</td>
<td>-0.19</td>
<td>23.64</td>
</tr>
<tr>
<td>2B1</td>
<td>π → 3p_z</td>
<td>-3.44</td>
<td>14.90</td>
</tr>
<tr>
<td>3A1</td>
<td>π → 4p_x, n → 3s</td>
<td>-0.41</td>
<td>26.75</td>
</tr>
<tr>
<td>3B1</td>
<td>π → 4s, π → 3s</td>
<td>1.81</td>
<td>19.21</td>
</tr>
<tr>
<td>1B2</td>
<td>n → 3p_y, n → 4p_y</td>
<td>-0.72</td>
<td>13.28</td>
</tr>
<tr>
<td>2A2</td>
<td>π → 4p_y, π → 3p_y</td>
<td>-0.58</td>
<td>14.00</td>
</tr>
<tr>
<td>4B1</td>
<td>n → 3p_x</td>
<td>-0.95</td>
<td>37.26</td>
</tr>
<tr>
<td>4A1</td>
<td>n → 3p_z</td>
<td>-2.79</td>
<td>17.01</td>
</tr>
<tr>
<td>5A1</td>
<td>π → 4p_x</td>
<td>-0.71</td>
<td>34.32</td>
</tr>
<tr>
<td>Triplet states</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1B1</td>
<td>π → 3s(OH*)</td>
<td>0.51</td>
<td>9.82</td>
</tr>
<tr>
<td></td>
<td>π → 4s</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1A2</td>
<td>π → 3p_y, π → 4p_y</td>
<td>-0.70</td>
<td>10.98</td>
</tr>
<tr>
<td>1A1</td>
<td>n → 3s(OH*)</td>
<td>0.52</td>
<td>11.96</td>
</tr>
<tr>
<td>2A1</td>
<td>π → 3p_x, π → 4p_x</td>
<td>-0.99</td>
<td>31.45</td>
</tr>
<tr>
<td>2B1</td>
<td>π → 3p_z</td>
<td>-3.26</td>
<td>14.53</td>
</tr>
<tr>
<td>3B1</td>
<td>π → 4s, π → 3s</td>
<td>1.66</td>
<td>19.66</td>
</tr>
<tr>
<td>1B2</td>
<td>n → 3p_y, n → 4p_y</td>
<td>-0.46</td>
<td>11.50</td>
</tr>
<tr>
<td>2A2</td>
<td>π → 4p_y, π → 3p_y</td>
<td>-0.58</td>
<td>13.97</td>
</tr>
<tr>
<td>3A1</td>
<td>n → 3p_x</td>
<td>-2.95</td>
<td>16.89</td>
</tr>
<tr>
<td>4B1</td>
<td>n → 3p_z</td>
<td>-0.98</td>
<td>36.16</td>
</tr>
<tr>
<td>4A1</td>
<td>π → 4p_x</td>
<td>-1.31</td>
<td>38.17</td>
</tr>
<tr>
<td>Ionized (Cation doublet) states</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1B1</td>
<td>π</td>
<td>-0.90</td>
<td>3.59</td>
</tr>
<tr>
<td>1A1</td>
<td>n</td>
<td>-0.73</td>
<td>4.44</td>
</tr>
<tr>
<td>1B2</td>
<td>σ</td>
<td>-1.11</td>
<td>4.51</td>
</tr>
</tbody>
</table>

### Usage of SelecCISOnly

1. Singlet B_{1u} states, V(\pi, \pi^*) and \pi-3d states of ethylene are calculated by the SAC-CI SD-R method with [4s2p1d2s] 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.

<table>
<thead>
<tr>
<th>Level</th>
<th>LevelOne</th>
<th>LevelTwo</th>
<th>LevelThree</th>
</tr>
</thead>
<tbody>
<tr>
<td>ground</td>
<td>2827</td>
<td>3556</td>
<td>5115</td>
</tr>
<tr>
<td>excited B$_{1u}$</td>
<td>1928</td>
<td>2469</td>
<td>4012</td>
</tr>
</tbody>
</table>

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 $\pi$-3d states of ethylene.

<table>
<thead>
<tr>
<th>State</th>
<th>Character</th>
<th>SECI</th>
<th>SAC-CI SD-R</th>
<th>Exptl.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>E(eV)</td>
<td>Oscillator strength</td>
<td>Second moment</td>
</tr>
<tr>
<td>B$_{1u}$</td>
<td>V($\pi, \pi^*$)</td>
<td>7.733</td>
<td>0.364</td>
<td>105.5</td>
</tr>
<tr>
<td>$\pi \rightarrow 3d\pi$</td>
<td>9.009</td>
<td>0.063</td>
<td>222.2</td>
<td>9.33</td>
</tr>
</tbody>
</table>

### 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:

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

<table>
<thead>
<tr>
<th>State</th>
<th>Character</th>
<th>SAC-CI SD-R</th>
<th>Exptl.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>E(eV)</td>
<td>Oscillator strength</td>
</tr>
<tr>
<td>Ground state</td>
<td>---</td>
<td>---</td>
<td>83.6</td>
</tr>
<tr>
<td>Singlet excited states</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A$_g$</td>
<td>$\pi \rightarrow 3p\pi$</td>
<td>8.223</td>
<td>0.0</td>
</tr>
<tr>
<td>B$_{1g}$</td>
<td>$\pi \rightarrow 3p\sigma$</td>
<td>7.878</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>$\sigma \rightarrow \pi^*$</td>
<td>8.942</td>
<td>0.0</td>
</tr>
</tbody>
</table>
Singlet, triplet and ionized states of ethylene are calculated by the SAC-CI SD-$R$ method. Details are same as Input 634.

1. 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.

<table>
<thead>
<tr>
<th>State</th>
<th>SAC-CI SD-$R$</th>
<th>Exptl.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LevelThree</td>
<td>LevelTwo</td>
</tr>
<tr>
<td>Dim. E(eV)</td>
<td>Dim. E(eV)</td>
<td>Dim. E(eV)</td>
</tr>
</tbody>
</table>

Ground state

<table>
<thead>
<tr>
<th>State</th>
<th>Dim.</th>
<th>E(eV)</th>
<th>Dim.</th>
<th>E(eV)</th>
<th>Dim.</th>
<th>E(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5115</td>
<td>---</td>
<td>---</td>
<td>3556</td>
<td>---</td>
<td>2827</td>
<td>---</td>
</tr>
</tbody>
</table>

Singlet states

<table>
<thead>
<tr>
<th>State</th>
<th>Dim.</th>
<th>E(eV)</th>
<th>Dim.</th>
<th>E(eV)</th>
<th>Dim.</th>
<th>E(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_g$</td>
<td>3599</td>
<td>8.223</td>
<td>2044</td>
<td>8.189</td>
<td>1511</td>
<td>8.155</td>
</tr>
<tr>
<td>$B_{1g}$</td>
<td>4234</td>
<td>7.878</td>
<td>3327</td>
<td>7.838</td>
<td>2874</td>
<td>7.796</td>
</tr>
<tr>
<td>$B_{2g}$</td>
<td>4420</td>
<td>7.901</td>
<td>3344</td>
<td>7.859</td>
<td>2838</td>
<td>7.821</td>
</tr>
</tbody>
</table>

Ionized states

<table>
<thead>
<tr>
<th>State</th>
<th>Dim.</th>
<th>E(eV)</th>
<th>Dim.</th>
<th>E(eV)</th>
<th>Dim.</th>
<th>E(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(3a_g)^{-1}$</td>
<td>14.676</td>
<td>0.923[b]</td>
<td>72.3</td>
<td>14.66</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$(1b_{3g})^{-1}$</td>
<td>13.008</td>
<td>0.932</td>
<td>71.8</td>
<td>12.85</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$(2b_{1u})^{-1}$</td>
<td>19.500</td>
<td>0.853</td>
<td>72.6</td>
<td>19.23</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$(1b_{2u})^{-1}$</td>
<td>16.176</td>
<td>0.886</td>
<td>72.8</td>
<td>15.87</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$(1b_{3u})^{-1}$</td>
<td>10.371</td>
<td>0.951</td>
<td>72.7</td>
<td>10.51</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

[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>
<thead>
<tr>
<th>Level</th>
<th>Singlet Energy</th>
<th>Triplet Energy</th>
<th>Ionized Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>B$_{3g}$</td>
<td>3953</td>
<td>9.836</td>
<td>2545</td>
</tr>
<tr>
<td>A$_{u}$</td>
<td>2107</td>
<td>8.890</td>
<td>1449</td>
</tr>
<tr>
<td>B$_{1u}$</td>
<td>4012</td>
<td>8.195</td>
<td>2469</td>
</tr>
<tr>
<td>B$_{2u}$</td>
<td>1400</td>
<td>8.919</td>
<td>876</td>
</tr>
<tr>
<td>B$_{3u}$</td>
<td>3389</td>
<td>7.235</td>
<td>2606</td>
</tr>
<tr>
<td>B$_{4u}$</td>
<td>1400</td>
<td>8.919</td>
<td>876</td>
</tr>
<tr>
<td>B$_{5u}$</td>
<td>3389</td>
<td>7.235</td>
<td>2606</td>
</tr>
</tbody>
</table>

**Triplet states**

<table>
<thead>
<tr>
<th>Level</th>
<th>Singlet Energy</th>
<th>Triplet Energy</th>
<th>Ionized Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>A$_{g}$</td>
<td>2729</td>
<td>8.060</td>
<td>1636</td>
</tr>
<tr>
<td>B$_{1g}$</td>
<td>5778</td>
<td>7.843</td>
<td>4217</td>
</tr>
<tr>
<td>B$_{2g}$</td>
<td>5932</td>
<td>7.839</td>
<td>4257</td>
</tr>
<tr>
<td>B$_{3g}$</td>
<td>6127</td>
<td>9.630</td>
<td>3679</td>
</tr>
<tr>
<td>A$_{u}$</td>
<td>2951</td>
<td>8.884</td>
<td>1725</td>
</tr>
<tr>
<td>B$_{1u}$</td>
<td>3139</td>
<td>4.518</td>
<td>2189</td>
</tr>
<tr>
<td>B$_{2u}$</td>
<td>1783</td>
<td>8.903</td>
<td>1050</td>
</tr>
<tr>
<td>B$_{3u}$</td>
<td>4519</td>
<td>7.123</td>
<td>3195</td>
</tr>
</tbody>
</table>

**Ionized states**

<table>
<thead>
<tr>
<th>Level</th>
<th>Singlet Energy</th>
<th>Triplet Energy</th>
<th>Ionized Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>A$_{g}$</td>
<td>330</td>
<td>14.676</td>
<td>322</td>
</tr>
<tr>
<td>B$_{3g}$</td>
<td>299</td>
<td>13.008</td>
<td>270</td>
</tr>
<tr>
<td>B$_{1u}$</td>
<td>312</td>
<td>19.500</td>
<td>283</td>
</tr>
<tr>
<td>B$_{2u}$</td>
<td>297</td>
<td>16.176</td>
<td>277</td>
</tr>
<tr>
<td>B$_{3u}$</td>
<td>210</td>
<td>10.371</td>
<td>197</td>
</tr>
</tbody>
</table>

**CPU time**

<table>
<thead>
<tr>
<th>Component</th>
<th>LevelOne</th>
<th>LevelTwo</th>
<th>LevelThree</th>
</tr>
</thead>
<tbody>
<tr>
<td>SCF(L502)</td>
<td>1.8s</td>
<td>1.8s</td>
<td>1.8s</td>
</tr>
<tr>
<td>ERI(L804)</td>
<td>4.6s</td>
<td>4.6s</td>
<td>4.6s</td>
</tr>
<tr>
<td>SAC-CI</td>
<td>542s</td>
<td>289s</td>
<td>194s</td>
</tr>
<tr>
<td>Energy</td>
<td>428s</td>
<td>223s</td>
<td>146s</td>
</tr>
<tr>
<td>Transition</td>
<td>114s</td>
<td>66s</td>
<td>48s</td>
</tr>
<tr>
<td>Density</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>9m12s</td>
<td>4m59s</td>
<td>3m24s</td>
</tr>
</tbody>
</table>

[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).

Table 8. Excitation, ionization, and electron-attachment energies of CO$_2$.

<table>
<thead>
<tr>
<th>State</th>
<th>Character</th>
<th>SAC-CI SD-R</th>
<th>Exptl.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>E(eV)</td>
<td>Oscillator strength</td>
</tr>
<tr>
<td>Ground state</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Singlet excited states</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Pi_g$</td>
<td>$\pi_g \rightarrow \sigma_g(R)^{[a]}$</td>
<td>9.06</td>
<td>--- $^{[b]}$</td>
</tr>
<tr>
<td>$\Sigma_u^-$</td>
<td>$\pi_g \rightarrow \pi_u$</td>
<td>9.36</td>
<td>--- $^{[b]}$</td>
</tr>
<tr>
<td>$\Delta_u$</td>
<td>$\pi_g \rightarrow \pi_u$</td>
<td>9.44</td>
<td>--- $^{[b]}$</td>
</tr>
<tr>
<td>$\Sigma_u^+$</td>
<td>$\pi_g \rightarrow \pi_u(R)$</td>
<td>11.31</td>
<td>0.12</td>
</tr>
<tr>
<td>$\Pi_u$</td>
<td>$\pi_g \rightarrow \sigma_u(R)$</td>
<td>11.42</td>
<td>0.02</td>
</tr>
<tr>
<td>Triplet states</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Sigma_u^+$</td>
<td>$\pi_g \rightarrow \pi_u$</td>
<td>8.37</td>
<td></td>
</tr>
<tr>
<td>$\Pi_g$</td>
<td>$\pi_g \rightarrow \sigma_g(R)$</td>
<td>8.96</td>
<td></td>
</tr>
<tr>
<td>$\Delta_u$</td>
<td>$\pi_g \rightarrow \pi_u$</td>
<td>9.94</td>
<td></td>
</tr>
<tr>
<td>$\Sigma_u^-$</td>
<td>$\pi_g \rightarrow \pi_u$</td>
<td>9.36</td>
<td></td>
</tr>
<tr>
<td>$\Pi_u$</td>
<td>$\pi_g \rightarrow \sigma_u(R)$</td>
<td>11.33</td>
<td></td>
</tr>
<tr>
<td>$\Sigma_g^+$</td>
<td>$\pi_u \rightarrow \pi_u$</td>
<td>11.90</td>
<td></td>
</tr>
<tr>
<td>$\Delta_g$</td>
<td>$\pi_u \rightarrow \pi_u$</td>
<td>12.75</td>
<td></td>
</tr>
<tr>
<td>Ionized states</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Pi_g$</td>
<td>$\pi_g$</td>
<td>13.56</td>
<td>0.93$^{[c]}$</td>
</tr>
<tr>
<td>$\Pi_u$</td>
<td>$\pi_u$</td>
<td>17.85</td>
<td>0.90</td>
</tr>
<tr>
<td>$\Sigma_u^+$</td>
<td>$\sigma_u^+$</td>
<td>18.08</td>
<td>0.91</td>
</tr>
<tr>
<td>$\Sigma_g^+$</td>
<td>$\sigma_g^+$</td>
<td>19.41</td>
<td>0.90</td>
</tr>
<tr>
<td>Electron attached states</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Sigma_g^+$</td>
<td>$\sigma_g^+$</td>
<td>0.13</td>
<td></td>
</tr>
<tr>
<td>$\Sigma_u^+$</td>
<td>$\sigma_u^+$</td>
<td>0.23</td>
<td></td>
</tr>
<tr>
<td>$\Pi_u$</td>
<td>$\pi_u$</td>
<td>0.22</td>
<td></td>
</tr>
<tr>
<td>$\Pi_g$</td>
<td>$\pi_g$</td>
<td>0.51</td>
<td></td>
</tr>
</tbody>
</table>

$^{[a]}$ (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$_2$.

<table>
<thead>
<tr>
<th>State</th>
<th>SAC-CI SD-R</th>
<th>Exptl.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LevelThree</td>
<td>LevelTwo</td>
</tr>
<tr>
<td></td>
<td>Dim.</td>
<td>E(eV)</td>
</tr>
<tr>
<td>Ground state</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6626</td>
<td>4589</td>
<td>3745</td>
</tr>
<tr>
<td>Singlet excited states</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Pi_g$</td>
<td>6173</td>
<td>9.057</td>
</tr>
<tr>
<td>$\Delta_u$</td>
<td>7492</td>
<td>9.437</td>
</tr>
<tr>
<td>$\Sigma_u^+$</td>
<td>7789</td>
<td>11.307</td>
</tr>
<tr>
<td>$\Pi_u$</td>
<td>6581</td>
<td>11.421</td>
</tr>
<tr>
<td>Triplet states</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Sigma_u^+$</td>
<td>8354</td>
<td>8.373</td>
</tr>
<tr>
<td>$\Pi_g$</td>
<td>9072</td>
<td>8.964</td>
</tr>
</tbody>
</table>

58
\[\Delta_u \quad 8020 \quad 8.944 \quad 5277 \quad 8.938 \quad 4308 \quad 8.971 \quad 8.8\]
\[\Sigma_u^- \quad 8020 \quad 9.360 \quad 5277 \quad 9.338 \quad 4308 \quad 9.397 \]
\[\Pi_u \quad 10753 \quad 11.332 \quad 7463 \quad 11.301 \quad 6060 \quad 11.272 \]
\[\Sigma_u^+ \quad 10403 \quad 11.895 \quad 6636 \quad 11.889 \quad 5192 \quad 11.875 \]
\[\Delta_g \quad 10403 \quad 12.749 \quad 6636 \quad 12.742 \quad 5192 \quad 12.725 \quad 12.4\]

**Ionized states**

\[
\begin{align*}
\Pi_g & : 445 \quad 13.555 \quad 423 \quad 13.522 \quad 417 \quad 13.489 \quad 13.78 \\
\Pi_u & : 443 \quad 17.846 \quad 423 \quad 17.816 \quad 426 \quad 18.023 \quad 18.08 \\
\Sigma_u^+ & : 501 \quad 19.413 \quad 458 \quad 19.387 \quad 445 \quad 19.360 \quad 19.40
\end{align*}
\]

**Electron attached states**

\[
\begin{align*}
\Sigma g^+ & : 1167 \quad 0.125 \quad 386 \quad 0.129 \quad 182 \quad 0.132 \\
\Sigma u^+ & : 249 \quad 0.231 \quad 69 \quad 0.232 \quad 53 \quad 0.232 \\
\Pi u & : 232 \quad 0.215 \quad 60 \quad 0.216 \quad 38 \quad 0.216 \\
\Pi g & : 253 \quad 0.506 \quad 71 \quad 0.506 \quad 49 \quad 0.507
\end{align*}
\]

**CPU time**

<table>
<thead>
<tr>
<th>Method</th>
<th>LevelOne</th>
<th>LevelTwo</th>
</tr>
</thead>
<tbody>
<tr>
<td>SCF[b]</td>
<td>2s</td>
<td>2s</td>
</tr>
<tr>
<td>ERI[c]</td>
<td>6s</td>
<td>6s</td>
</tr>
<tr>
<td>SAC-CI</td>
<td>14m29s</td>
<td>7m49s</td>
</tr>
<tr>
<td>Total</td>
<td>14m41s</td>
<td>8m 1s</td>
</tr>
</tbody>
</table>

[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.**

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>NSol</th>
<th>Before selection</th>
<th>After selection</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>LevelOne</td>
<td>LevelTwo</td>
</tr>
<tr>
<td>A_g(SAC)</td>
<td>1</td>
<td>5920901</td>
<td>27395</td>
</tr>
<tr>
<td>B_{1u}</td>
<td>4</td>
<td>5916248</td>
<td>62118</td>
</tr>
<tr>
<td>B_{3u}</td>
<td>4</td>
<td>5916092</td>
<td>58771</td>
</tr>
<tr>
<td>B_{3u}</td>
<td>1</td>
<td>4876572</td>
<td>24353</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>State</th>
<th>Main configuration</th>
<th>Nature</th>
<th>Eex (eV)</th>
<th>f(Pol) (au)</th>
<th>Excitation (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1B_{1u}</td>
<td>(5b_{3u} \rightarrow 4b_{2g})-(2a_u \rightarrow 4b_{1g})</td>
<td>\pi \rightarrow \pi^*</td>
<td>1.77</td>
<td>0.00(x)</td>
<td>1.98(Q_x; very weak)</td>
</tr>
</tbody>
</table>
1B_{3u} \quad (5b_{3u} \rightarrow 4b_{1g})-(2a_u \rightarrow 4b_{2g}) \quad \pi \rightarrow \pi^* \quad 2.25 \quad 0.00(y) \quad 2.42(Q_y;\text{very weak})

2B_{1u} \quad (2a_u \rightarrow 4b_{1g})+(5b_{3u} \rightarrow 4b_{2g}) \quad \pi \rightarrow \pi^* \quad 3.58 \quad 1.18(x) \quad 3.33(B;\text{strong})

\quad - (4b_{3u} \rightarrow 4b_{2g})

2B_{3u} \quad (2a_u \rightarrow 4b_{2g})+(5b_{3u} \rightarrow 4b_{1g}) \quad \pi \rightarrow \pi^* \quad 3.71 \quad 1.69(y) \quad 3.65(N;broad)

3B_{1u} \quad (4b_{3u} \rightarrow 4b_{2g}) \quad \pi \rightarrow \pi^* \quad 4.14 \quad 0.78(x) \quad 4.25-4.67(L;weak)

3B_{2u} \quad (4b_{3u} \rightarrow 4b_{1g}) \quad \pi \rightarrow \pi^* \quad 4.33 \quad 0.27(y) \quad 4.25-4.67(L;weak)

1B_{3u} \quad (7b_{2u} \rightarrow 4b_{1g}) \quad n \rightarrow \pi^* \quad 4.42 \quad 0.00(z) \quad 4.25-4.67(L;weak)

4B_{3u} \quad (3b_{3u} \rightarrow 4b_{1g}) \quad \pi \rightarrow \pi^* \quad 4.85 \quad 0.30(y) \quad 5.0-5.5(M;weak)

4B_{1u} \quad (3b_{3u} \rightarrow 4b_{2g}) \quad \pi \rightarrow \pi^* \quad 4.92 \quad 0.41(x) \quad 5.0-5.5(M;weak)

[a]"LevelOne" denotes accuracy of ETthreS2=1.d-5 and ETthreR2=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:

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

<table>
<thead>
<tr>
<th>State</th>
<th>SAC-CI</th>
<th>Exptl.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LevelOne</td>
<td>LevelTwo</td>
</tr>
<tr>
<td></td>
<td>E_{ex} (eV)</td>
<td>f(Pol) (au)</td>
</tr>
<tr>
<td>1B_{1u}</td>
<td>1.77</td>
<td>0.00</td>
</tr>
<tr>
<td>1B_{2u}</td>
<td>2.25</td>
<td>0.00</td>
</tr>
<tr>
<td>2B_{1u}</td>
<td>3.58</td>
<td>1.18</td>
</tr>
<tr>
<td>2B_{2u}</td>
<td>3.71</td>
<td>1.69</td>
</tr>
<tr>
<td>3B_{1u}</td>
<td>4.14</td>
<td>0.78</td>
</tr>
<tr>
<td>3B_{2u}</td>
<td>4.33</td>
<td>0.27</td>
</tr>
<tr>
<td>1B_{3u}</td>
<td>4.42</td>
<td>0.00</td>
</tr>
<tr>
<td>4B_{2u}</td>
<td>4.85</td>
<td>0.30</td>
</tr>
<tr>
<td>4B_{1u}</td>
<td>4.92</td>
<td>0.41</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>CPU time[a]</th>
</tr>
</thead>
<tbody>
<tr>
<td>SCF(L502)</td>
</tr>
<tr>
<td>ERI(L804)</td>
</tr>
<tr>
<td>SAC-CI</td>
</tr>
<tr>
<td>Energy</td>
</tr>
<tr>
<td>Transition Density</td>
</tr>
<tr>
<td>Total</td>
</tr>
</tbody>
</table>

[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.

<table>
<thead>
<tr>
<th>Method</th>
<th>R(H-C) (Angstrom)</th>
<th>R(C-F) (Angstrom)</th>
<th>∠ HCF (degree)</th>
<th>$T_e/T_0$ [a] (eV)</th>
<th>Total energy (au)</th>
</tr>
</thead>
<tbody>
<tr>
<td>X A' ground state</td>
<td>1.126</td>
<td>1.320</td>
<td>102.2</td>
<td>-</td>
<td>-138.09945(-138.09999)</td>
</tr>
<tr>
<td>Exptl.</td>
<td>1.138</td>
<td>1.305</td>
<td>104.1</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>A A&quot; excited state</td>
<td>1.102</td>
<td>1.311</td>
<td>123.5</td>
<td>2.380</td>
<td>-138.01199(-138.01184)</td>
</tr>
<tr>
<td>Exptl.</td>
<td>1.063</td>
<td>1.308</td>
<td>123.8</td>
<td>2.142</td>
<td>-</td>
</tr>
</tbody>
</table>

[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 NH2, an open-shell molecule; $X^2B_1$ (ground) and $A^2A_1$ (excited) states of NH2 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 (NH2-) 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.

### Table 14. Optimized structure and energy of the $X^2B_1$ (ground) and $A^2A_1$ (excited) states of NH2.

<table>
<thead>
<tr>
<th>Method</th>
<th>R(N-H) (Angstrom)</th>
<th>∠ HNH (degree)</th>
<th>$T_e/T_0$ [a] (eV)</th>
<th>Total energy (au)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X^2B_1$ ground state</td>
<td>1.028</td>
<td>103.5</td>
<td>-</td>
<td>-55.75497 (-55.75488)</td>
</tr>
<tr>
<td>D95(d,p)</td>
<td>1.022</td>
<td>103.6</td>
<td>-</td>
<td>-55.78815 (-55.78805)</td>
</tr>
<tr>
<td>cc-pVTZ</td>
<td>1.024 (1.025)</td>
<td>103.36 (102.9)</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Exptl.</td>
<td>0.997</td>
<td>145.1</td>
<td>1.473</td>
<td>-55.70082 (-55.70094)</td>
</tr>
<tr>
<td>$A^2A_1$ excited state</td>
<td>0.978</td>
<td>143.7</td>
<td>1.356</td>
<td>-55.73831 (-55.73827)</td>
</tr>
<tr>
<td>D95(d,p)</td>
<td>0.976</td>
<td>144</td>
<td>1.271</td>
<td>-</td>
</tr>
<tr>
<td>cc-pVTZ</td>
<td>0.976</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Exptl.</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

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

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### 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.

Table 15. Dimension, excitation energy, and CPU time in different level of approximation for MoS$_4$ dianion.

<table>
<thead>
<tr>
<th>State</th>
<th>SAC-CI SD-R</th>
<th>Exptl.$^a$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LevelThree</td>
<td>LevelTwo</td>
</tr>
<tr>
<td></td>
<td>Dim. E(eV)</td>
<td>Dim. E(eV)</td>
</tr>
<tr>
<td>Ground state</td>
<td></td>
<td></td>
</tr>
<tr>
<td>23896</td>
<td>---</td>
<td>12995</td>
</tr>
<tr>
<td>Singlet excited states</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1T$_1$</td>
<td>27654</td>
<td>19814</td>
</tr>
<tr>
<td>1T$_2$</td>
<td>27654</td>
<td>19814</td>
</tr>
<tr>
<td>1E</td>
<td>26710</td>
<td>15135</td>
</tr>
<tr>
<td>2T$_1$</td>
<td>27654</td>
<td>19814</td>
</tr>
<tr>
<td>2T$_2$</td>
<td>27654</td>
<td>19814</td>
</tr>
<tr>
<td></td>
<td>3.598</td>
<td>3.537</td>
</tr>
<tr>
<td></td>
<td>3.756</td>
<td>3.693</td>
</tr>
</tbody>
</table>

CPU time

<table>
<thead>
<tr>
<th></th>
<th>LevelTwo (Without Degeneracy)</th>
<th>Exptl.$^a$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Dim. E(eV)</td>
<td></td>
</tr>
<tr>
<td>Ground state</td>
<td>10694</td>
<td>---</td>
</tr>
<tr>
<td>Singlet excited states</td>
<td>15267,15115,15151$^{b}$</td>
<td>2.281,2.333,2.275</td>
</tr>
<tr>
<td>1T$_1$</td>
<td>15267,15115,15151</td>
<td>2.723,2.762,2.712</td>
</tr>
<tr>
<td>1T$_2$</td>
<td>15267,15115,15151</td>
<td>3.582,3.560</td>
</tr>
<tr>
<td>1E</td>
<td>15267,15115,15151</td>
<td>3.580,3.587,3.577</td>
</tr>
<tr>
<td>2T$_1$</td>
<td>15267,15115,15151</td>
<td>3.748,3.751,3.745</td>
</tr>
<tr>
<td>2T$_2$</td>
<td>15267,15115,15151</td>
<td>ca.3.91</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>SCF(L502)</th>
<th>ERI(L804)</th>
<th>SAC-CI</th>
<th>Energy</th>
<th>Transition density</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1s</td>
<td>4s</td>
<td>46m21s</td>
<td>2510s</td>
<td>271s</td>
</tr>
<tr>
<td></td>
<td>4s</td>
<td>4s</td>
<td></td>
<td>1140s</td>
<td>127s</td>
</tr>
<tr>
<td></td>
<td>13m12s</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>13m21s</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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.

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

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

<table>
<thead>
<tr>
<th>Character</th>
<th>SAC-CI SD-R</th>
<th>Exptl.</th>
</tr>
</thead>
<tbody>
<tr>
<td>State</td>
<td>Dim.</td>
<td>E(eV)</td>
</tr>
<tr>
<td>Ground state</td>
<td>55363</td>
<td></td>
</tr>
<tr>
<td>Singlet excited states</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A_u</td>
<td>n^+</td>
<td>π</td>
</tr>
<tr>
<td>B_g</td>
<td>n^-</td>
<td>π</td>
</tr>
<tr>
<td>Triplet states</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A_u</td>
<td>n^+</td>
<td>π</td>
</tr>
<tr>
<td>Ionized states</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A_g</td>
<td>n^+</td>
<td>2716</td>
</tr>
<tr>
<td>B_u</td>
<td>n^-</td>
<td>2719</td>
</tr>
<tr>
<td>B_g</td>
<td>Π</td>
<td>1961</td>
</tr>
<tr>
<td>A_u</td>
<td>Π</td>
<td>1959</td>
</tr>
</tbody>
</table>

[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.

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

<table>
<thead>
<tr>
<th>State</th>
<th>Character</th>
<th>SAC-CI SD-R</th>
<th>Exptl.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LevelThree</td>
<td>LevelTwo</td>
<td>LevelOne</td>
</tr>
<tr>
<td>State</td>
<td>Dim.</td>
<td>E(eV)</td>
<td>Dim.</td>
</tr>
<tr>
<td>Ground state</td>
<td>55363</td>
<td>---</td>
<td>24399</td>
</tr>
<tr>
<td>Singlet states</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A_u</td>
<td>24551</td>
<td>3.03</td>
<td>14110</td>
</tr>
<tr>
<td>B_g</td>
<td>28298</td>
<td>4.45</td>
<td>16177</td>
</tr>
<tr>
<td>Triplet states</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A_u</td>
<td>30328</td>
<td>2.64</td>
<td>15629</td>
</tr>
<tr>
<td>Ionized states</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A_g</td>
<td>2716</td>
<td>10.58</td>
<td>2343</td>
</tr>
<tr>
<td>B_u</td>
<td>2719</td>
<td>12.384</td>
<td>2336</td>
</tr>
<tr>
<td>A_u</td>
<td>1959</td>
<td>15.683</td>
<td>1668</td>
</tr>
</tbody>
</table>

CPU time[a]
### 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.

<table>
<thead>
<tr>
<th></th>
<th>CMO</th>
<th>LMO</th>
<th>full linked term[a]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Ground state</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dim.</td>
<td>17102 (C\text{\textsubscript{1}})</td>
<td>5925 (C\text{\textsubscript{1}})</td>
<td>51359 (C\text{\textsubscript{1}})</td>
</tr>
<tr>
<td>E(corr.)</td>
<td>-0.34644</td>
<td>-0.38384</td>
<td>-0.38884</td>
</tr>
<tr>
<td>E(total)</td>
<td>-191.04976</td>
<td>-191.08715</td>
<td>-191.09215</td>
</tr>
<tr>
<td><strong>Excited state</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dim.</td>
<td>7076 (C\text{\textsubscript{1}})</td>
<td>5064 (C\text{\textsubscript{1}})</td>
<td>51359 (C\text{\textsubscript{1}})</td>
</tr>
<tr>
<td>E(total)</td>
<td>-190.90577</td>
<td>-190.94187</td>
<td>-190.94288</td>
</tr>
<tr>
<td>Excitation energy (eV)</td>
<td>3.92</td>
<td>3.95</td>
<td>4.06</td>
</tr>
</tbody>
</table>

[a] Unlinked terms were selected with normal thresholds.

### 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\textsubscript{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\textsuperscript{+} 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\textsubscript{2} with 6-31G*.

<table>
<thead>
<tr>
<th>State</th>
<th>SAC-CI-NV</th>
<th>EOM-CC</th>
<th>Full-CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Singlet</td>
<td>Full #1 #2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A\textsubscript{1}</td>
<td>0.0</td>
<td>.....</td>
<td>.....</td>
</tr>
<tr>
<td></td>
<td>5.844</td>
<td>5.871</td>
<td>5.796</td>
</tr>
</tbody>
</table>
9.120  9.109  9.111  9.120  9.053
B_1   1.668  1.669  1.692  1.668  1.679
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

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; ET=ET2=CThreULS2G=CThreULR1=CThreULR2=0.0

#2: Unlinked terms are same as #1 and further selection is performed with default thresholds; ET=1.d-6, ET2=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].

<table>
<thead>
<tr>
<th>State</th>
<th>SAC-CI-NV</th>
<th>SAC-CI-V</th>
<th>CC-LRT</th>
<th>full-CI</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Full</td>
<td>#1</td>
<td>#2</td>
<td>#1</td>
</tr>
<tr>
<td>Σ+</td>
<td>0.000</td>
<td>......</td>
<td>......</td>
<td>0.000</td>
</tr>
<tr>
<td>Π</td>
<td>3.261</td>
<td>3.265</td>
<td>3.271</td>
<td>3.262</td>
</tr>
<tr>
<td></td>
<td>3.261</td>
<td>3.265</td>
<td>3.271</td>
<td>3.262</td>
</tr>
</tbody>
</table>

#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.

<table>
<thead>
<tr>
<th>R (au)</th>
<th>SAC Energy (au)</th>
<th>Σ+</th>
<th>Π+</th>
<th>SAC-CI Energy (au)</th>
<th>Σ+</th>
<th>Π+</th>
</tr>
</thead>
</table>
Table 22. Spectroscopic constants of the singlet states of Li₂,[a]

<table>
<thead>
<tr>
<th>Source</th>
<th>$T_e$ ($T_o$)</th>
<th>$R_e$</th>
<th>$D_e$</th>
<th>$\omega_e$</th>
<th>$\omega_e\chi_e$</th>
<th>$B_e$</th>
<th>$\alpha_e$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi\Sigma_g^+$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D95(d)</td>
<td>0.0</td>
<td>2.695</td>
<td>8212</td>
<td>350.0</td>
<td>2.59</td>
<td>0.663</td>
<td>0.006</td>
</tr>
<tr>
<td>cc-pVTZ</td>
<td>0.0</td>
<td>2.689</td>
<td>8767</td>
<td>346.3</td>
<td>2.49</td>
<td>0.666</td>
<td>0.007</td>
</tr>
<tr>
<td>Exptl.[b]</td>
<td>0.0</td>
<td>2.673</td>
<td>8541</td>
<td>351.4</td>
<td>2.58</td>
<td>0.672</td>
<td>0.007</td>
</tr>
<tr>
<td>$A\Sigma_u^+$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D95(d)</td>
<td>1.674(1.680)</td>
<td>3.149</td>
<td>9086</td>
<td>259.8</td>
<td>1.50</td>
<td>0.486</td>
<td>0.005</td>
</tr>
<tr>
<td>cc-pVTZ</td>
<td>1.715(1.721)</td>
<td>3.124</td>
<td>9304</td>
<td>254.6</td>
<td>1.66</td>
<td>0.493</td>
<td>0.006</td>
</tr>
<tr>
<td>Exptl.[b]</td>
<td>1.74</td>
<td>3.108</td>
<td>8940</td>
<td>255.4</td>
<td>1.58</td>
<td>0.498</td>
<td>0.005</td>
</tr>
<tr>
<td>(9469)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$B\Pi_u$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D95(d)</td>
<td>2.665(2.671)</td>
<td>3.035</td>
<td>2019</td>
<td>254.0</td>
<td>4.24</td>
<td>0.523</td>
<td>0.010</td>
</tr>
<tr>
<td>cc-pVTZ</td>
<td>2.550(2.555)</td>
<td>2.956</td>
<td>3287</td>
<td>270.3</td>
<td>3.11</td>
<td>0.551</td>
<td>0.008</td>
</tr>
<tr>
<td>Exptl.[b]</td>
<td>2.53</td>
<td>2.935</td>
<td>3102</td>
<td>270.1</td>
<td>2.67</td>
<td>0.558</td>
<td>0.008</td>
</tr>
<tr>
<td>$1\Pi_g$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D95(d)</td>
<td>2.654(2.670)</td>
<td>4.152</td>
<td>1181</td>
<td>84.6</td>
<td>1.87</td>
<td>0.279</td>
<td>0.011</td>
</tr>
<tr>
<td>cc-pVTZ</td>
<td>2.697(2.713)</td>
<td>4.052</td>
<td>1381</td>
<td>95.6</td>
<td>1.78</td>
<td>0.293</td>
<td>0.009</td>
</tr>
<tr>
<td>Exptl.[b]</td>
<td></td>
<td>2.560</td>
<td>1412</td>
<td>96.7</td>
<td>1.89</td>
<td>0.297</td>
<td>0.009</td>
</tr>
<tr>
<td>$2\Sigma_g^+$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D95(d)</td>
<td>2.525(2.537)</td>
<td>3.466</td>
<td>3113</td>
<td>157.1</td>
<td>0.320</td>
<td>0.401</td>
<td>0.010</td>
</tr>
<tr>
<td>cc-pVTZ</td>
<td>2.497(2.508)</td>
<td>3.516</td>
<td>3892</td>
<td>161.1</td>
<td>...</td>
<td>0.390</td>
<td>0.004</td>
</tr>
</tbody>
</table>

[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. $D_e$, $\omega_e$, $\omega_e\chi_e$, $B_e$, and $\alpha_e$ are in cm$^{-1}$.


### 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 N₂, 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).


Table 23. Energies (in au) of the singlet to septet states of N₂ (R=1.09768 Å) calculated by the SAC-CI SD-R method.

<table>
<thead>
<tr>
<th>Singlet states</th>
<th>SAC-CI-V</th>
<th>$\Delta$ (mH)</th>
<th>SAC-CI-NV</th>
<th>$\Delta$ (mH)</th>
<th>full-CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma_g^+$</td>
<td>-108.54462</td>
<td>-5.15</td>
<td>-108.54351</td>
<td>-4.04</td>
<td>-108.53947</td>
</tr>
<tr>
<td>$\Delta_g$</td>
<td>-108.27285</td>
<td>49.95</td>
<td>-108.27284</td>
<td>49.96</td>
<td>-108.32280</td>
</tr>
<tr>
<td>$\Pi_g$</td>
<td>-108.63761</td>
<td>1.14</td>
<td>-108.63711</td>
<td>1.64</td>
<td>-108.63875</td>
</tr>
<tr>
<td>State</td>
<td>Σ</td>
<td>Δ</td>
<td>Π</td>
<td>Average Discrepancy</td>
<td></td>
</tr>
<tr>
<td>------------</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>---------------------</td>
<td></td>
</tr>
<tr>
<td>Triplet states</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Σ^+</td>
<td>-108.55950</td>
<td>-108.58832</td>
<td>4.89</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Δ^+</td>
<td>-108.55405</td>
<td>-108.58712</td>
<td>4.97</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Π^+</td>
<td>-108.55405</td>
<td>-108.58712</td>
<td>4.97</td>
<td></td>
<td></td>
</tr>
<tr>
<td>average discrepancy</td>
<td>4.89</td>
<td>4.97</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CationDoublet states</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Σ^+</td>
<td>-108.43598</td>
<td>-108.43497</td>
<td>52.96</td>
<td></td>
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</tr>
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<td>1490</td>
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<td>1119</td>
<td>48775</td>
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<tr>
<td>** Sextet**</td>
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</table>

Table 24. Dimensions of SAC-CI and full-CI for singlet to septet states of $\text{N}_2$ ($R=1.09768$ Å); SD-R without selection and general-R with selection.
### 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.


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.

<table>
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<tr>
<th></th>
<th>SAC-CI-V general-$R$</th>
<th>$\Delta$ (mhartree)</th>
<th>full-CI (hartree)</th>
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<td>$\Delta_g$</td>
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<td>$\Sigma_g^-$</td>
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<td>-108.48710</td>
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<td>Triplet states</td>
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average discrepancy 8.22
Quartet states
\[ \Sigma_u^- \] -108.12426 1.22 -108.12548
\[ \Delta_u \] -108.07742 1.19 -108.07861
\[ \Pi_u \] -108.05902 2.81 -108.06183
\[ \Sigma_u^- \] -108.05438 1.92 -108.05630
\[ \Pi_u \] -108.02149 2.91 -108.02440
\[ \Sigma_g^+ \] -108.01471 1.31 -108.01602
\[ \Delta_g \] -107.96637 1.05 -107.96742
\[ \Sigma_g^- \] -107.94626 1.44 -107.94770
average discrepancy 1.73
Quintet states
\[ \Pi_g \] -108.40114 1.34 -108.40248
\[ \Sigma_g^+ \] -108.38025 1.08 -108.38133
\[ \Sigma_g^- \] -108.37014 2.18 -108.37232
\[ \Pi_g \] -108.29198 1.83 -108.29381
\[ \Sigma_u^+ \] -108.25350 1.44 -108.25494
\[ \Sigma_g^+ \] -108.21902 1.34 -108.22036
\[ \Delta_g \] -108.20674 1.28 -108.20802
\[ \Pi_g \] -108.18380 3.35 -108.18715
\[ \Delta_g \] -108.17161 1.32 -108.17293
\[ \Pi_g \] -108.15289 3.94 -108.15683
average discrepancy 1.91
Sextet states
\[ \Pi_g \] -107.81807 1.53 -107.81960
\[ \Sigma_g^+ \] -107.80069 0.70 -107.80139
\[ \Sigma_g^- \] -107.68979 1.23 -107.69102
average discrepancy 1.15
Septet states
\[ \Sigma_g^+ \] -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 \( C^4 \Delta \) 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. \( C^4 \Delta \) 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. \( T_0 \)).
5. Details of the spectroscopic constants are given in the paper.

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<th>Excitation level</th>
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<th>Without selection[a]</th>
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<td></td>
<td>( R_e ) (A)</td>
<td>( T_e / T_0 ) (eV)</td>
<td>Total energy(au)</td>
</tr>
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<td></td>
<td></td>
<td></td>
<td>( R_e ) (A)</td>
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</table>

Table 26. Optimized structure and energy of the ground \( X^1 \Sigma_g^+ \) and singlet \( C^4 \Delta \) states of BH.
### 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 $X^1\Sigma_g^+$ and $B^3\Sigma_u^-$ 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 $B^3\Sigma_u^-$ state, since it is described by three-electron process.

### Input 649 ###   Force at vertical excited states
1. Internal coordinate forces in the singlet \( (n \rightarrow \pi^+) \), triplet \( (n \rightarrow \pi^+) \), and ionized states \( (n \rightarrow \cdot) \) 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>
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<th>State</th>
<th>Nature</th>
<th>Force (Hartree/Bohr or radian)</th>
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</thead>
<tbody>
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<td>( n \rightarrow \pi^+ )</td>
<td>dE/dR(NO) = 0.0414</td>
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<tr>
<td></td>
<td></td>
<td>dE/dR(NH) = -0.0062</td>
</tr>
<tr>
<td></td>
<td></td>
<td>dE/dA(HNO) = 0.0236</td>
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<tr>
<td>( T_1 )</td>
<td>( n \rightarrow \pi^+ )</td>
<td>dE/dR(NO) = 0.0273</td>
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<tr>
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<td></td>
<td>dE/dR(NH) = -0.0136</td>
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<tr>
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<td></td>
<td>dE/dA(HNO) = 0.0335</td>
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<tr>
<td>( I_1 )</td>
<td>( n \rightarrow \cdot )</td>
<td>dE/dR(NO) = -0.0863</td>
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<td>dE/dR(NH) = 0.0064</td>
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<tr>
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<td></td>
<td>dE/dA(HNO) = 0.0418</td>
</tr>
</tbody>
</table>

\(^{[a]}\) 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 \( S_0 \rightarrow S_1 \) excitation were observed:

\[ dR(NO) = +0.030 \text{ (Ang.)}, \quad dR(NH) = -0.026 \text{ (Ang.)}, \quad \text{and} \quad dA(HNO) = +7.7 \text{ (deg.)}. \]

(F.W. Dalby, Can. J. Phys. 36 (1958) 1336.)

### Input 650 ### H\(_2\)CO: Singlet, triplet, Ionized: All properties

1. Singlet, triplet, ionized, and electron-attached states of H\(_2\)CO 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\(_2\)CO are calculated.

<table>
<thead>
<tr>
<th>State</th>
<th>Character</th>
<th>Excitation energy (eV)</th>
<th>Dipole moment (au)</th>
<th>Oscillator Strength</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>SAC-CI</td>
<td>Exptl.</td>
<td>SAC-CI</td>
</tr>
<tr>
<td>1A(_1)</td>
<td>ground</td>
<td>0.00</td>
<td>0.939</td>
<td>0.913</td>
</tr>
<tr>
<td>1A(_2)</td>
<td>( n \rightarrow \pi^+ )</td>
<td>4.18</td>
<td>4.1, 4.2</td>
<td>0.510</td>
</tr>
<tr>
<td>1B(_2)</td>
<td>( n \rightarrow 3s )</td>
<td>7.01</td>
<td>7.091, 7.13</td>
<td>-1.131</td>
</tr>
<tr>
<td>2A(_1)</td>
<td>( n \rightarrow 3p_y )</td>
<td>7.95</td>
<td>8.14</td>
<td>0.061</td>
</tr>
<tr>
<td>2B(_2)</td>
<td>( n \rightarrow 3p_z )</td>
<td>7.95</td>
<td>7.97, 8.00</td>
<td>0.700</td>
</tr>
</tbody>
</table>
Table 31. Excitation energy and dipole moment of the triplet states of HCHO.

<table>
<thead>
<tr>
<th>State</th>
<th>Character</th>
<th>Excitation energy (eV)</th>
<th>Dipole moment (au)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2A2</td>
<td>n \rightarrow 3p_x</td>
<td>8.19</td>
<td>0.303</td>
</tr>
<tr>
<td>3B2</td>
<td>n \rightarrow 3s</td>
<td>9.35</td>
<td>2.067</td>
</tr>
<tr>
<td>3A1</td>
<td>n \rightarrow 3p_y</td>
<td>9.54</td>
<td>1.025</td>
</tr>
<tr>
<td>1B1</td>
<td>5a_1 \rightarrow \pi^*</td>
<td>9.59</td>
<td>0.203</td>
</tr>
<tr>
<td>3A2</td>
<td>n \rightarrow 3p_z</td>
<td>9.66</td>
<td>0.740</td>
</tr>
<tr>
<td>4A1</td>
<td>\pi \rightarrow \pi^*</td>
<td>10.33</td>
<td>10.7</td>
</tr>
<tr>
<td>2B1</td>
<td>\pi \rightarrow 3s</td>
<td>10.84</td>
<td>10.7</td>
</tr>
<tr>
<td>3B1</td>
<td>n \rightarrow 3p_z</td>
<td>11.80</td>
<td>11.6-11.9</td>
</tr>
</tbody>
</table>

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

Table 32. Ionization Potential of HCHO.

<table>
<thead>
<tr>
<th>State</th>
<th>Character</th>
<th>Ionization Potential (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1B2</td>
<td>n</td>
<td>10.47</td>
</tr>
<tr>
<td>1B1</td>
<td>\pi</td>
<td>14.33</td>
</tr>
<tr>
<td>1A1</td>
<td>5a_1</td>
<td>15.80</td>
</tr>
<tr>
<td>2B2</td>
<td>1b_2</td>
<td>17.14</td>
</tr>
<tr>
<td>2A1</td>
<td>4a_1</td>
<td>21.34</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>State</th>
<th>Character</th>
<th>Second moment (au)</th>
<th>Diamagnetic Susceptibilities</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>&lt;x^2&gt;</td>
<td>&lt;y^2&gt;</td>
</tr>
<tr>
<td>1A1</td>
<td>ground</td>
<td>8.8</td>
<td>15.3</td>
</tr>
<tr>
<td>1A2</td>
<td>n \rightarrow \pi^*</td>
<td>10.6</td>
<td>14.3</td>
</tr>
<tr>
<td>1B2</td>
<td>\pi \rightarrow 3s</td>
<td>20.2</td>
<td>26.2</td>
</tr>
<tr>
<td>2A1</td>
<td>n \rightarrow 3p_y</td>
<td>18.7</td>
<td>46.1</td>
</tr>
<tr>
<td>2B2</td>
<td>n \rightarrow 3p_z</td>
<td>20.7</td>
<td>25.4</td>
</tr>
</tbody>
</table>

73
### Input 651 ### H₂CO 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 34. Second moment and diamagnetic susceptibilities of the triplet states of HCHO.

<table>
<thead>
<tr>
<th>State</th>
<th>Character</th>
<th>Second moment (au)</th>
<th>Diamagnetic Susceptibilities</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>&lt;x²&gt;</td>
<td>&lt;y²&gt;</td>
</tr>
<tr>
<td>1A₂</td>
<td>n → π⁺</td>
<td>10.6</td>
<td>14.2</td>
</tr>
<tr>
<td>1A₁</td>
<td>π → π⁺</td>
<td>9.1</td>
<td>15.3</td>
</tr>
<tr>
<td>1B₂</td>
<td>π → 3s</td>
<td>18.8</td>
<td>25.4</td>
</tr>
<tr>
<td>2B₂</td>
<td>n → 3p_z</td>
<td>19.8</td>
<td>24.5</td>
</tr>
<tr>
<td>2A₁</td>
<td>n → 3p_y</td>
<td>18.1</td>
<td>44.6</td>
</tr>
<tr>
<td>2A₂</td>
<td>n → 3p_x</td>
<td>43.8</td>
<td>24.4</td>
</tr>
<tr>
<td>1B₁</td>
<td>5a₁ → π⁺</td>
<td>10.2</td>
<td>15.2</td>
</tr>
<tr>
<td>3B₂</td>
<td>π → 3s</td>
<td>17.4</td>
<td>22.9</td>
</tr>
<tr>
<td>3A₁</td>
<td>n → 3p_y</td>
<td>17.7</td>
<td>42.7</td>
</tr>
<tr>
<td>3A₂</td>
<td>1b₂ → π⁺</td>
<td>11.1</td>
<td>14.0</td>
</tr>
<tr>
<td>2B₁</td>
<td>π → 3s</td>
<td>18.6</td>
<td>26.8</td>
</tr>
<tr>
<td>3B₁</td>
<td>n → 3p_z</td>
<td>18.1</td>
<td>24.9</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Method</th>
<th>R(HC) (A)</th>
<th>R(CO) (A)</th>
<th>∠HCH (degree)</th>
<th>∠OOP [a]</th>
<th>T_e/T₀ [b] (eV)</th>
<th>Total energy (au)</th>
</tr>
</thead>
<tbody>
<tr>
<td>X¹A'</td>
<td>1.108</td>
<td>1.216</td>
<td>116.4</td>
<td>-</td>
<td>-</td>
<td>-114.22024</td>
</tr>
<tr>
<td>Exptl.</td>
<td>1.101</td>
<td>1.203</td>
<td>116.3</td>
<td>0.0</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>A¹A'&quot;</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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

- **Method**: SAC-CI, Exptl.
- **R(HC)**: 1.108, 1.101 A
- **R(CO)**: 1.216, 1.203 A
- **∠HCH**: 116.4, 116.3°
- **∠OOP [a]**: -
- **Tₑ/T₀ [b]**: -114.22024 eV
- **Total energy** (au): -
### Hyperfine Splitting Constants

1. Hyperfine splitting constants (hfsc) of CH₃, H₂O⁺, and NH₂ radicals are calculated.
2. D95 basis sets are used and the dimension of AO basis is 16, 14, and 14 for CH₃, H₂O⁺, and NH₂, respectively. All SCF MOs are included in the active space (default for SpinDensity).

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

<table>
<thead>
<tr>
<th>Molecule</th>
<th>State</th>
<th>Total energy (au)</th>
<th>Atom</th>
<th>hfsc (Gauss)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>SAC-CI</td>
<td>Exptl.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>GTO[^a]</td>
<td>STO[^b]</td>
</tr>
<tr>
<td>CH₃⁺</td>
<td>A₂</td>
<td>-39.65860</td>
<td>C</td>
<td>32.4</td>
<td>25.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H</td>
<td>-27.9</td>
<td>-29.6</td>
</tr>
<tr>
<td>H₂O⁺</td>
<td>B₁</td>
<td>-75.73233</td>
<td>O</td>
<td>-22.2</td>
<td>-26.0</td>
</tr>
<tr>
<td>NH₂</td>
<td>B₁</td>
<td>-55.66341</td>
<td>N</td>
<td>8.0</td>
<td>7.3</td>
</tr>
</tbody>
</table>

[^a]: Input 652
Thresholds and algorithm for calculating spin density are different from these references.

### 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.

<table>
<thead>
<tr>
<th>State</th>
<th>Dimension</th>
<th>Character</th>
<th>E (eV)</th>
<th>Oscillator strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ground</td>
<td>17138</td>
<td>V</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>Excited A₁</td>
<td>19818</td>
<td>3d Rydberg</td>
<td>6.321</td>
<td>0.0000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>7.570</td>
<td>0.0617</td>
</tr>
<tr>
<td>CPU time (sec)</td>
<td>Separated</td>
<td>Non-separated</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>33m34s</td>
<td>21m39s</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**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.

<table>
<thead>
<tr>
<th>Sub-keyword</th>
<th>SAC-NV</th>
<th>SAC-CI-V</th>
<th>SAC-CI-NV</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>ITERATIVE</td>
<td>sac</td>
<td>sciv</td>
<td>scinv</td>
<td>cid</td>
</tr>
<tr>
<td>DIRECT</td>
<td>dsac</td>
<td>das</td>
<td>dnas</td>
<td>das</td>
</tr>
</tbody>
</table>

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.

   \[ &\text{CNTL SINGLET(S-INITIAL PROPERTY) &END} \]

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

   \[ &\text{CNTL IONIZED(GENERAL-R SAC-CI-NV DIRECT) &END} \]

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.

   \[ &\text{CNTL QUARTET(SAC-CI-NV D-INITIAL HFSC) &END} \]

=========================================================================
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

   \[ &\text{CNTL SINGLET &END} \]

is terminated, the restart should be done with the input

   \[ &\text{CNTL SINGLET RESTART &END} \]

=========================================================================

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, 1, 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,

<table>
<thead>
<tr>
<th>ISYM</th>
<th>C1</th>
<th>C1</th>
<th>C1</th>
<th>C2</th>
<th>C2</th>
<th>C2v</th>
<th>C2h</th>
<th>D2</th>
<th>D2h</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>a</td>
<td>a_a</td>
<td>a'</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
</tr>
<tr>
<td>2</td>
<td>a_u</td>
<td>a''</td>
<td>b</td>
<td>a_b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>a</td>
</tr>
<tr>
<td>3</td>
<td>b</td>
<td>a_u</td>
<td>a</td>
<td>b</td>
<td>a</td>
<td>a</td>
<td>b</td>
<td>b</td>
<td>b</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
</tr>
<tr>
<td>5</td>
<td>b</td>
<td>a</td>
<td>a</td>
<td>b</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
</tr>
<tr>
<td>6</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
</tr>
<tr>
<td>7</td>
<td>b</td>
<td>a</td>
<td>a</td>
<td>b</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
</tr>
<tr>
<td>8</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
<td>b</td>
</tr>
</tbody>
</table>
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

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, 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,
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, /

* Step ci matrix *  

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)
&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), ifsk1(I), ifsch1(I), ifscs1(I),
ifschh(O), ifscss(O)
AGSUM: ifscg(I), ifsgk(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.
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 *

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,

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

<table>
<thead>
<tr>
<th>integral type</th>
<th>TERM1</th>
<th>TERM2</th>
<th>TERM3</th>
<th>TERM4</th>
<th>Default</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt; 0</td>
<td>H</td>
<td>S(1)*S(1)&gt;</td>
<td>ON/OFF</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;S(1)</td>
<td>H</td>
<td>S(1)*S(1)&gt;</td>
<td>ON/OFF</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;S(2)</td>
<td>H</td>
<td>S(1)*S(1)&gt;</td>
<td>ON/OFF</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;S(1)</td>
<td>H</td>
<td>S(1)*S(2)&gt;</td>
<td>---</td>
<td>ON/OFF</td>
<td>---</td>
</tr>
<tr>
<td>&lt;S(2)</td>
<td>H</td>
<td>S(1)*S(2)&gt;</td>
<td>---</td>
<td>ON/OFF</td>
<td>---</td>
</tr>
<tr>
<td>&lt;S(2)</td>
<td>H</td>
<td>S(2)*S(2)&gt;</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;S(1)</td>
<td>H</td>
<td>S(1)*S(1)*S(1)&gt;</td>
<td>---</td>
<td>---</td>
<td>ON/OFF</td>
</tr>
<tr>
<td>&lt;S(2)</td>
<td>H</td>
<td>S(1)*S(1)*S(1)&gt;</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;S(2)</td>
<td>H</td>
<td>S(1)*S(1)*S(2)&gt;</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;S(2)</td>
<td>H</td>
<td>S(1)*S(1)*S(1)*S(1)&gt;</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
</tbody>
</table>
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
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)

<table>
<thead>
<tr>
<th>integral type</th>
<th>options to activate</th>
<th>TERM1</th>
<th>TERM2</th>
<th>TERM3</th>
<th>TERM4</th>
<th>Default</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;R(1)</td>
<td>H</td>
<td>R(1)*S(1)&gt;</td>
<td>ON-OFF</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;R(2)</td>
<td>H</td>
<td>R(1)*S(1)&gt;</td>
<td>ON-OFF</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;R(1)</td>
<td>H</td>
<td>R(1)*S(2)&gt;</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;R(2)</td>
<td>H</td>
<td>R(1)*S(2)&gt;</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;R(1)</td>
<td>H</td>
<td>R(2)*S(1)&gt;</td>
<td>---</td>
<td>ON/OFF</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;R(2)</td>
<td>H</td>
<td>R(2)*S(1)&gt;</td>
<td>---</td>
<td>ON/OFF</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;R(2)</td>
<td>H</td>
<td>R(2)*S(2)&gt;</td>
<td>---</td>
<td>---</td>
<td>ON/OFF</td>
<td>---</td>
</tr>
<tr>
<td>&lt;R(1)</td>
<td>H</td>
<td>R(1)*S(1)*S(1)&gt;</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;R(2)</td>
<td>H</td>
<td>R(1)*S(1)*S(1)&gt;</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;R(2)</td>
<td>H</td>
<td>R(2)*S(1)*S(1)&gt;</td>
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<tr>
<td>&lt;R(2)</td>
<td>H</td>
<td>R(1)*S(1)*S(2)&gt;</td>
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<td>---</td>
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</tr>
<tr>
<td>&lt;R(2)</td>
<td>H</td>
<td>R(2)*S(1)*S(2)&gt;</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;S(2)</td>
<td>H</td>
<td>R(1)*S(1)*S(1)*S(1)&gt;</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;R(1)</td>
<td>H</td>
<td>exp(S)&gt;</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt;R(2)</td>
<td>H</td>
<td>exp(S)&gt;</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>&lt; 0</td>
<td>H</td>
<td>R(1)*S(1)&gt;</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
</tbody>
</table>

(CMAXG=0.005)
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--

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
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 damping 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 $|0\rangle$ 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 $|0\rangle$ within variable space.
         0 ... No
         1 ... Yes
         (Default: 1)

EPSQ   : Density convergence criterion
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>
<thead>
<tr>
<th>Method</th>
<th>Step</th>
<th>#SCIV#</th>
<th>#SCINV#</th>
<th>#DAS# and #DNAS#</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>IN2ND</td>
<td>INHFC</td>
<td>INHFC</td>
<td>ISCRPT</td>
</tr>
<tr>
<td>-----------------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>--------</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

(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-$R$
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 *

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

<table>
<thead>
<tr>
<th>Istep</th>
<th>Excitation operators</th>
<th>Hamiltonian matrix</th>
<th>Overlap matrix</th>
<th>Unlinked integrals</th>
<th>Solutions</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>iflabb(I)</td>
<td>ifhmx2(I)</td>
<td>ifsmx2(I)</td>
<td>---</td>
<td>ifsol2(O)</td>
</tr>
<tr>
<td>4</td>
<td>iflbre(I)</td>
<td>ifhmre(I)</td>
<td>ifsmre(I)</td>
<td>---</td>
<td>ifslre(O)</td>
</tr>
<tr>
<td>5,6</td>
<td>iflabe(I)</td>
<td>ifhmx3(I)</td>
<td>ifsmx3(I)</td>
<td>ifumx3(I)</td>
<td>ifsol3(O)</td>
</tr>
</tbody>
</table>

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.

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

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 *

Step for diagonalization of SAC-CI-NV (non-variational) matrix (non-symmetric) by iterative procedure

The method is described in

You can include $|0\rangle$ within variable space and solve SAC-CI vectors including pseudo-SAC wf. in the solution space.

See ** Remarks ** in #SCIV#

Namelist Group -- &SCINV --

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>INHFC</td>
<td>Include Hartree-Fock configuration $</td>
</tr>
<tr>
<td></td>
<td>0 ... No</td>
</tr>
<tr>
<td></td>
<td>1 ... Yes</td>
</tr>
<tr>
<td></td>
<td>(Note : This option corresponds to WITHHF of DNAS, etc.)</td>
</tr>
<tr>
<td></td>
<td>(Default: 1)</td>
</tr>
<tr>
<td>ISCRPT</td>
<td>Include script-S part.</td>
</tr>
<tr>
<td></td>
<td>0 ... No</td>
</tr>
<tr>
<td></td>
<td>1 ... Yes</td>
</tr>
<tr>
<td></td>
<td>** Note **</td>
</tr>
<tr>
<td></td>
<td>Except for singlet A1 excited state, this option is not used. When SAC-CI gradients are selected, script-S-part is not included.</td>
</tr>
<tr>
<td></td>
<td>(Default: 0)</td>
</tr>
<tr>
<td>EPSQ</td>
<td>Density convergence criterion</td>
</tr>
<tr>
<td></td>
<td>(Default: 1.0d^-4)</td>
</tr>
<tr>
<td>MIT</td>
<td>Maximum number of iteration per solution</td>
</tr>
<tr>
<td></td>
<td>(Default: 35)</td>
</tr>
<tr>
<td>IPROC</td>
<td>Print out iterative procedure</td>
</tr>
<tr>
<td></td>
<td>0 ... No</td>
</tr>
<tr>
<td></td>
<td>1 ... Yes</td>
</tr>
<tr>
<td></td>
<td>(Default: 0)</td>
</tr>
<tr>
<td>FPR</td>
<td>Threshold for printing out SAC-CI coefficients</td>
</tr>
<tr>
<td></td>
<td>(Default: 1.0d-1)</td>
</tr>
<tr>
<td>IPRINT</td>
<td>Level of printing, see &amp;PRES for details.</td>
</tr>
<tr>
<td></td>
<td>(Default: 0)</td>
</tr>
</tbody>
</table>
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), ifsych(I), ifscss(I), ifscit(I),
  ifscun(I),
  ifscsn(O)
AGSUM: ifsccg(I), ifscgk(I)

high-spin and general-R
  ifcom(I), iflabe(I), ifhm3x(I), ifsmx3(I), ifumx3(I), ifsl3n(O)

### *

* Step Diagnas *

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-CT'.
( 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, 

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: 'SCRPTS')

ICALHI : Calculation of higher-order unlinked terms R(2)*S(2) in SAC-CI.  
=0 : No
=1 : Yes
(Default: 0)

THREECC : 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 in step #DENS#. Property operator integrals are evaluated with PRISM algorithm (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).

#GSUM#

* Step 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
(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.
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.
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
(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 AGSUM)/6-31G Opt

gamestry 1'
molecule specification

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

INPUT(I), OUTPUT(O), WORK(W) file information
* 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-\textit{R}
\textit{ifsccm(I)}, \textit{ifscsv(I: SAC-CI-V)}, \textit{ifscsn(I: SAC-CI-NV)}

general-\textit{R}
\textit{ifcom(I)}, \textit{ifsol3(I: SAC-CI-V)}, \textit{ifsl3n(I: SAC-CI-NV)}, \textit{ifsols(I)}, \textit{iflabe(I)}, \textit{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)**

**-----------------------------------------------------------------------------------**

**#COMCG#**

* Step common change *

**Step to rewrite information in the common file**

**-----------------------------------------------------------------------------------**

Namelist group -&PRINT-

  **i=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(O), WORK(W) file information

ifscm(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)

110
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----------------------> |
| <--------NOCC2 ---> | <------NVAC2 ---> |

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.

\[ \begin{align*}
&=0: \text{Do not selection for D (quartet and quintet) or T (sextet and septet)} \\
&=1: \text{Do selection for D or T (Default: 1)}
\end{align*} \]

**NTGENH**
Type of generating higher-order terms

\[ \begin{align*}
&=0: \text{Exponentially-generation scheme is used.} \\
&=1: \text{All the higher-order terms up to triples (for singlet and triplet states) or quadruples (for ionized, anionized, quartet states) are generated for selection. (Default: 0)}
\end{align*} \]

**ISKIPH**
Type of selecting higher-order terms for calculating unlinked integrals in case of NTGENH=1.

\[ \begin{align*}
&=0: \text{small CI is done.} \\
&=1: \text{small CI is skipped. (Default: 0)}
\end{align*} \]

Note:
ISTEP controls the function of step #GHPRES#.

\[ \begin{align*}
\text{istep} = 1: \text{Generation of excitation operators for reference-CI} \\
\text{istep} = 2: \text{Generation of SD-CI (A-CI or B-CI) excitation operators}
\end{align*} \]

Sample input

\[ \begin{align*}
&PRES \\
&\text{JCALC(1,5)=1, JCALC(2,5)=1, JCALC(3,5)=1, JCALC(4,5)=1,} \\
&\text{JCALC(1,7)=1, JCALC(2,7)=1, JCALC(3,7)=1, JCALC(4,7)=1,} \\
&\text{JCALC(1,8)=1, JCALC(2,8)=1, JCALC(3,8)=1, JCALC(4,8)=1,} \\
&\text{JCALC(1,10)=1, JCALC(2,10)=1, JCALC(3,10)=1, JCALC(4,10)=1,} \\
&\text{MSOL(1,5)=1, MSOL(2,5)=1, MSOL(3,5)=1, MSOL(4,5)=1,} \\
&\text{MSOL(1,7)=1, MSOL(2,7)=1, MSOL(3,7)=1, MSOL(4,7)=1,} \\
&\text{MSOL(1,8)=1, MSOL(2,8)=1, MSOL(3,8)=1, MSOL(4,8)=1,} \\
&\text{MSOL(1,10)=1, MSOL(2,10)=1, MSOL(3,10)=1, MSOL(4,10)=1,} \\
&\text{ISEL(5)=2, ISEL(7)=2, ISEL(8)=2, ISEL(10)=2,} \\
&\text{ESELG=1.d-5,} \\
&\text{ESELE(5)=1.d-6, ESELE(7)=1.d-6, ESELE(8)=1.d-6, ESELE(10)=1.d-6,} \\
&\text{CMAIN(5)=0.1, CMAIN(7)=0.1, CMAIN(8)=0.1, CMAIN(10)=0.1,} \\
&\text{CSPIN(5)=1, CSPIN(7)=1, CSPIN(8)=1, CSPIN(10)=1,} \\
&/ \\
&\&GHPRES \\
&\text{MAXEXC(5)=4, MAXEXC(7)=4, MAXEXC(8)=3, MAXEXC(10)=3,}
\end{align*} \]
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),  ifcsy(O), iflabr(O), iflbra(O), iflabb(O), iflab(a(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 \( R = A \cdot B \)
(Default: \( \text{THRMB1(KSTATE)} = 0.04, \text{THRMB2(KSTATE)} = 0.04 \))

\( \text{THMMB1(KSTATE)}, \text{THMMB2(KSTATE)} \)
Thresholds for \( B(1) \) and \( B(2) \) operators, respectively, for
exponential generation of higher-order terms by \( R = A \cdot A \cdot B \)
(Default: \( \text{THMMB1(KSTATE)} = 0.1, \text{THMMB2(KSTATE)} = 0.1 \))

\( \text{ISELEG} \)
Perturbation selection is done for higher-order linked terms.
=0 : without perturbation selection
=1 : with perturbation selection
(Default: 1)

\( \text{ESELEG(KSTATE)} \)
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 \( \text{CMAIN(KSTATE)} \) and
\( \text{ISEL(KSTATE)} \), respectively. (See namelist &PRES)
\( \text{ISEL(KSTATE)} \) should be 1.

\( \text{THRUI3(KSTATE)}, \text{THRUI4(KSTATE)}, \text{THRUI5(KSTATE)}, \text{THRUI6(KSTATE)} : \)
Threshold of generating unlinked integrals for the
unlinked operators \( R(3) = A(1) \cdot B(2), A(2) \cdot B(1), R(4) = A(2) \cdot B(2), R(5) = A(2) \cdot A(2) \cdot B(1), A(1) \cdot A(2) \cdot B(2), R(6) = A(2) \cdot A(2) \cdot B(2) \)
(Default: \( \text{THRUI3(KSTATE)} = 0.1, \text{THRUI4(KSTATE)} = 0.1, \text{THRUI5(KSTATE)} = 0.1, \text{THRUI6(KSTATE)} = 0.1 \))

** Note **
For example, the \( R(5) = A(2) \cdot A(2) \cdot B(1) \) operator whose
products of reference CI coefficients \( a(2) \cdot a(2) \cdot b(1) \) are
larger than \( \text{THRUI5(KSTATE)} \) is used to generate the unlinked
terms \( R(5) \cdot S(2) \).

\( \text{MXRED} \)
Unit of working space for storing selected operators
(Default: Automatically determined.)

** Note **
\( \text{MXRED} \) should be increased when the number of high-order
excitation operators exceed this limit.

\( \text{MXRED2} \)
Unit of working space for storing excitation operators
before perturbation selection
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), iflab(I), iflabl(I), ifsol1(I), ifsol2(I),
iflabe(O),
iflbt1(W), iflbt2(W), iflbt3(W)

*****************************************************************************

* Step MEGI *

Hamiltonian matrix, overlap matrix, and unlinked integrals for SAC-CI general-R and high-spin calculations.

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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=1d-8, IPRINT=0, /

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

ifcom(I), ifscmo(I), ifscer(I), ifscsy(I),

<table>
<thead>
<tr>
<th>istep</th>
<th>Excitation operators</th>
<th>Hamiltonian matrix</th>
<th>overlap matrix</th>
<th>unlinked integrals</th>
<th>solutions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>iflabr(I)</td>
<td>ifhmx1(O)</td>
<td>ifsmx1(O)</td>
<td>- -</td>
<td>- -</td>
</tr>
<tr>
<td>2</td>
<td>iflabb(I)</td>
<td>ifhmx2(O)</td>
<td>ifsmx2(O)</td>
<td>- -</td>
<td>- -</td>
</tr>
<tr>
<td>4</td>
<td>iflibra(I)</td>
<td>ifhmre(O)</td>
<td>ifsmre(O)</td>
<td>- -</td>
<td>- -</td>
</tr>
<tr>
<td>5</td>
<td>iflabe(I)</td>
<td>ifhmx3(O)</td>
<td>ifsmx3(O)</td>
<td>- -</td>
<td>- -</td>
</tr>
<tr>
<td>6</td>
<td>iflab(I)</td>
<td>- -</td>
<td>- -</td>
<td>ifumx3(I)</td>
<td>ifsol1(I)</td>
</tr>
</tbody>
</table>
<pre><code>                  | iflabs(I)            |                    |                |                   | ifsol2(I) |
                  |                      |                    |                |                   | ifsols(I) |
</code></pre>

* 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:

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 *       #ZVECT#       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,ifscsi,ifscsy,ifsci,ifsci,
          ifsh24, ifsh02, ifscka(4), ifscgk(4),
          ifschoh(9,4), ifscsh(9,4),ifscit(9,4), ifscrc(9,4), ifscsn(9,4),
          ifscx(9,4), ifscsv(9,4),ifscsn(9,4),ifscno(9,4), ifscsd(9,4),
          ifsckx(9,4), ifscsv(9,4), ifscsn(9,4), ifscno(9,4),
          ifscg1, ifscgr(9,4)
common /ifscf2/ ifsck1(4), ifscsh1(9,4), ifscs1(9,4)
common /ifscf3/ ifflag
common /ifscf5/ ifscg1
common /ifscf7/ ifsccl
common /ififif/ 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>

<table>
<thead>
<tr>
<th>File name</th>
<th>File numbers</th>
<th>Contents and structure (C2v case)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ifscer</td>
<td>3503</td>
<td>E : Orbital energies</td>
</tr>
<tr>
<td></td>
<td></td>
<td>R : MO electron repulsion integrals</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(MOERI)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Llim : Lower limit of active MOs</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Iulim: Upper limit of active MOs</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Symmetrically non-zero MOERI's are</td>
</tr>
</tbody>
</table>
stored.
\[(E(i),i=1,Nbf)\]
\[Nmo,Nbasis,Llim,Iulim, \ \ (itype)\]
\[(R(i),i=1,N)\]

\[<O:BPRES/I:PRES,CIMX,ULINT,ZVECIT>\]

ifcsy 3506 Information for symmetric reduction of molecular integrals
\[<O:BPRES/I:PRES,CIMX,ULINT,ZVECIT,EDM>\]

ifsh24 301 Hamiltonian matrix element
\[<S(I)|H|S(I)>\]
and overlap matrix element
\[<S(2)|S(1)>\]
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
\[i=1,j=1 \ \ \ ...H1,...;H01,H02,...; \]
\[...I,...;HI,...; \]
else \[E \ ...H1,...;I,...; \]
\[...HI,...; \]

\[<O:CIMX/I:SCIV,SCINV,DAS,DNAS,ZVECIT,EDM>\]

ifscun(j,i) \ ((i+6)*500+ 60+j \) Unlinked terms containing
\[<R(I)|H|R(I)> \]
for SAC-CI-V and NV
\[E \ ...I,...;UI,...; \]

\[<O:ULINT/I:SCIV,SCINV,DAS,DNAS>\]

#############################################################################
###    check point file    ###
#############################################################################

ifsccl 340 NAT34 information

ifscceg 341 General computational information in Gsum step
File structure is identical to ifscclm.

\[<O:GSUM/I:ALL STEPS>\]

ifscgk(i) 342+i Excitation operators in Gsum step
File structure is identical to ifsccka(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
ifscul 342  Flags for S2- operators for calculating unlinked terms

ifflag 3500  Job status of SAC/SAC-CI calculation

ifsccm 3501  General computational information

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)

ifscfi 3504  Information of MOERI file
            nferi,nblk,kount,nunit

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)

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;...
ifscss(j,i)  (i+6)*500+ 30+j  Overlap matrix elements between linked
  
G,E   ...SII...;..I,J...;...SII... 

<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 
  
Temat, (Cm(i),i=1,Ndt) 
  
Temat : 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.
### 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.

```plaintext
common /ghfile/ ifcom, ifmo, iferi, iflabb(8), iflab(8), iflabs,
    iflbr(8), iflbe(8), iflb(8), iflbt1(8), iflbt2(8), iflbt3(8),
    ifhm(8), ifhm2(8), ifhm3(8), ifhmre(8), ifsmx1(8), ifsmx2(8),
```

---

occupations 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

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(i, j), ii=1,Nbf), jj=1,Nmo):...

---

### III-B. File numbers of SAC/SAC-CI general-$R$ and high-spin calculation

- **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):...
  
- **ifscd(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(i, j), ii=1,Nbf), jj=1,Nmo):...

---

#### scratch file (xxx.scr) ###

- **ifsciw**  3507  
  Work unit

- **ifsck1(i)**  \((i+6)*500+10\)  
  Work unit for saving excitation operators
  
- **ifsch1(j,i)**  \((i+6)*500+20+j\)  
  Work unit for saving diagonal elements
  of Hamiltonian matrix

- **ifscs1(j,i)**  \((i+6)*500+30+j\)  
  Work unit for saving diagonal elements
  of Overlap matrix
Access to each file is shown as `<O:Output/I:Input/W:Working unit>`

<table>
<thead>
<tr>
<th>File name</th>
<th>File numbers</th>
<th>Contents and structure (C2v case)</th>
</tr>
</thead>
<tbody>
<tr>
<td>iferi</td>
<td>3503</td>
<td>MOERI file (same as ifscer of SD-R) Used in ZVecIt</td>
</tr>
<tr>
<td>ifscsy</td>
<td>3506</td>
<td>Same as SD-R Used in ZVecIt</td>
</tr>
<tr>
<td>ifhmx1(j)</td>
<td>(i+6)*500+360+j</td>
<td>Hamiltonian matrix elements of reference-CI</td>
</tr>
<tr>
<td>ifhmre(j)</td>
<td>(i+6)*500+470+j</td>
<td>Hamiltonian matrix elements of reference-EGCI</td>
</tr>
<tr>
<td>ifhmx2(j)</td>
<td>(i+6)*500+400+j</td>
<td>Hamiltonian matrix elements of singles and doubles</td>
</tr>
<tr>
<td>ifhmx3(j)</td>
<td>(i+6)*500+20+j</td>
<td>Hamiltonian matrix elements of triples and higher</td>
</tr>
<tr>
<td>ifumx3(j)</td>
<td>(i+6)*500+60+j</td>
<td>Hamiltonian matrix elements between linked and unlinked terms of SAC-CI high-spin and general-R</td>
</tr>
<tr>
<td>ifusx3(j)</td>
<td>(i+6)*500+340+j</td>
<td>Overlap matrix elements between linked and unlinked</td>
</tr>
</tbody>
</table>
terms of SAC-CI general-R
...I,J,...UIJ,...I,J,...UIJ,...

<O:MEGI/I:SCIV,SCINV,DAS,DNAS>

#############################
###     check point file    ###
#############################

ifcom 3507
(IOFCOM)
<O:GHPRES/I:ALL STEPS>

General computational information of
SAC-CI high-spin and general-R
Used during geometry optimization

ifmo 3502
(IOMO)
<O:MEGI,GHDENS,ZVECIT>

MO file (same as ifscmo in SD-R)
Used in ZVecIt

ifscfi 3504
(IOSCFI)
<O:MEGI,GHDENS,ZVECIT>

Same as SD-R
Used in ZVecIt

iflabb(j) (i+6)*500+390+j
(iflaba(j)
(IOSCKB(j))
<O:GHPRES/I:EGOP,MEGI,SCIV,SCINV,DAS,DNAS,ZVECIT>

Single and double excitation operators (A- and B-operators)
...Singles...Doubles...
for singlet-type operators)
Used during geometry optimization

iflabr(j) (i+6)*500+350+j
(iflbra(j)
(IOSCKR(j))
<O:GHPRES/I:EGOP,MEGI,DAS,ZVECIT>

Single and double excitation operators of reference-CI
...Singles...Doubles...
for singlet-type operators)
Used during geometry optimization

iflabe(j) (i+6)*500+10+j
(IOSCKA(j)) ifscka(j)
(IOLABE) iflabe(EGKSym)
<O:EGOP/I:MEGI,SCIV,SCINV,DAS,DNAS,ZVECIT,EDM>

Excitation operators of SAC-CI high-spin and general-R
...Singles...Doubles...Triples...
Used during geometry optimization

iflbre(j) (i+6)*500+460+j
<IOLABE) iflabe(EGKSym)
<O:EGOP/I:MEGI,SCIV,SCINV,DAS,DNAS,ZVECIT>

Excitation operators of reference-EGCI (small active space)
...Singles...Doubles...Triples...
...Quadruples...

ifsmx1(j) (i+6)*500+370+j
(ifsmra(j)
<O:MEGI/I:GHPRES,EGOP,DAS>

Overlap matrix elements of reference-CI
...SII...I,J...SIJ...
for singlet-type operators)
ifsmre(j)    (i+6)*500+480+j    Overlap matrix elements of reference-EGCI
            ..SIi...;IJ...;...SIJ...;I...;
            ..SIJ...
    <O:MEGI/I:EGOP,DAS>

ifsmx2(j)    (i+6)*500+410+j    Overlap matrix elements of singles and doubles
            ..SIi...;IJ...;...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...;IJ...;...SIJ...;I...;
            ..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 ifscrd
    <O:GHDENS>
ifini3(j) (i+6)*500+490+j <O:SCIV/I:SCIV> Initial vectors for iterative diagonalization

iflabs 3497 Excitation operators of SAC ground state (transferred from SAC-CI SD-R)
(IOLABS) ifscgk(1) Used in ZVecIt and Ov.11
<1:MEGI,SATEI,ZVECIT,EDM>

ifsols 3498 SAC-NV solution (transferred from SAC-CI SD-R)
(IOSOLS) ifscgk(1) Used in ZVecIt and Ov.11
<1:MEGI,SATEI,ZVECIT>

ifsss 3499 Overlap matrix of SAC (transferred from SAC-CI SD-R)
(IOSMXS) ifscgk(1) Used in ZVecIt and Ov.11
<1:MEGI,SATEI,ZVECIT>

###########################
###  scratch file (xxx.scr)  ###
###########################

ifscwk(4) 3521-3524 Work unit
<1:EGOP,SCIV,SCINV>

ifscwi(8) 3511-3518 Work unit
<1: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>

<table>
<thead>
<tr>
<th>File name</th>
<th>Contents and structure</th>
</tr>
</thead>
</table>

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.

\[ \text{IOSCKR}(j) \quad \text{iflabr(KSym)} \]
\[ \text{IOSCKB}(j) \quad \text{iflabb(KSym)} \]
\[ \text{IOSCKA}(j) \quad \text{iflabe(KSym)} \]

\[ \text{IOFCOM} \quad \text{ifcom} \]

Common block /GGHFIL/

### File Numbers defined/transfered in ZVecIt (Subroutine ZGHfio)

<table>
<thead>
<tr>
<th>Block</th>
<th>Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>IOMO</td>
<td>ifmo</td>
</tr>
<tr>
<td>IOERI</td>
<td>iferi</td>
</tr>
<tr>
<td>IOSCSY</td>
<td>ifscsy</td>
</tr>
<tr>
<td>IOSCFI</td>
<td>ifscfi</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Block</th>
<th>Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>IOSH24</td>
<td>JOSH24</td>
</tr>
<tr>
<td>IOSCUL</td>
<td>JOSCUL</td>
</tr>
<tr>
<td>IOLABS</td>
<td>JOLABS</td>
</tr>
<tr>
<td>IOHMXS</td>
<td>JOHMXS</td>
</tr>
<tr>
<td>IOHMX2</td>
<td>ifhmx2(EGKSym)</td>
</tr>
<tr>
<td>IOHMX3</td>
<td>ifhmx3(EGKSym)</td>
</tr>
<tr>
<td>IOMO</td>
<td>ifmo</td>
</tr>
<tr>
<td>IOSOLS</td>
<td>ifsols</td>
</tr>
<tr>
<td>IOSMXS</td>
<td>ifsss</td>
</tr>
<tr>
<td>IOSOL3</td>
<td>ifsol3(EGKSym)</td>
</tr>
<tr>
<td>IOSL3N</td>
<td>ifsl3n(EGKSym)</td>
</tr>
<tr>
<td>IOLABE</td>
<td>JOSCKA(EGKSym)</td>
</tr>
<tr>
<td>IOSCKX</td>
<td>JOSCGR(EGKSym)</td>
</tr>
<tr>
<td>IORDR3</td>
<td>JORdR3(EGSym)</td>
</tr>
<tr>
<td>IORDR4</td>
<td>JORdR4(EGSym)</td>
</tr>
<tr>
<td>IORDRH</td>
<td>JORdRH(EGSym)</td>
</tr>
<tr>
<td>IBucZv</td>
<td>CPSAC Z-vectors</td>
</tr>
</tbody>
</table>

Information of Common blocks
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

\[
\text{SAC-CI}=(\text{keyword1, keyword2, keyword3,\ldots}).
\]

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

\[
\begin{align*}
\text{SAC-CI} & = (\text{keyword1, keyword2,\ldots}, \text{Singlet}=(\text{keyword3, keyword4,\ldots}), \\
& \quad \text{Triplet}=(\text{keyword5, keyword6,\ldots}) \\
& \quad \text{Sextet}=(\text{keyword7, keyword8,\ldots}), \\
& \quad \text{Septet}=(\text{keyword9, keyword10,\ldots})
\end{align*}
\]

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.

\[
\begin{align*}
\text{SAC-CI options} & \quad \longrightarrow \quad \text{Array in core} \quad \longrightarrow \quad \text{Array in RWF} \quad \longrightarrow \quad \text{MyIOp} \\
\#\text{PrcSAC#} & \quad \#\text{SavSCI#} \quad \#\text{SACTrIOp#} \\
\mid \text{--------------------- L1 ---------------------} \mid \quad \mid \text{-----------------Link923-----------------} \mid
\end{align*}
\]

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

<table>
<thead>
<tr>
<th>Array Element</th>
<th>: SAC-CI Keywords</th>
<th>and size</th>
<th>: and sub-keywords</th>
<th>: Comment</th>
<th>: Translation (---&gt;)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimension ISACCI(10,8)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>==== Singlet State ====</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ISACCI(1,1)</td>
<td>Singlet=Nstate=N</td>
<td></td>
<td></td>
<td></td>
<td>(=\text{Number of Solutions for singlet states})</td>
</tr>
<tr>
<td>ISACCI(2,1)</td>
<td>Singlet=Nstate=(N-------)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ISACCI(3,1)</td>
<td>Singlet=Nstate=(-N------)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ISACCI(4,1)</td>
<td>Singlet=Nstate=(--N-----)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ISACCI(5,1)</td>
<td>Singlet=Nstate=(---N----)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ISACCI(6,1)</td>
<td>Singlet=Nstate=(----N---)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ISACCI(7,1)</td>
<td>Singlet=Nstate=(-----N--)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ISACCI(8,1)</td>
<td>Singlet=Nstate=(------N-)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ISACCI(9,1)</td>
<td>Singlet=Nstate=(-------N)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

--- Triplet State ---

| ISACCI(1,1) | Triplet=Nstate=N |
| 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 ==== Number of Solutions for anion-doublet

| ISACCI(1,4) | AnionDoublet=Nstate=N |
| 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 ==== Number of Solutions for quartet states

| ISACCI(1,5) | Quartet=Nstate=N |
| 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) |

==== Quintet ==== Number of Solutions for quintet states

| ISACCI(1,6) | Quintet=Nstate=N |
| ISACCI(2,6) | Quintet=Nstate=(N-------) |
| 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 |
| 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 |
| 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= |
| 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 |
SAACLMO(11) MaxItLin=N
SAACLMO(12) Omega=val
SAACLMO(13) CutOffDIIS=val
SAACLMO(14) CutOffDIISZvec=val
SAACLMO(15) TransitionFrom=SpinState=
               Singlet/Triplet/CationDoublet/AnionDoublet/
               Quintet/Quartet/Sextet/Septet ---> 1/2/3/4/5/6/7/8
SAACLMO(16) TransitionFrom=Symmetry=N
SAACLMO(17) TransitionFrom=Root=N
SAACLMO(18) MaxEgOp=N
SAACLMO(19) PrintOperator
SAACLMO(20) PrintNaturalOrbital
SAACLMO(21) PrintDensityMatrix
SAACLMO(22) CThreEgABAOp=A1Op=val
SAACLMO(23) CThreEgABAOp=A2Op=val
SAACLMO(24) CThreEgAABAOp=A1Op=val
SAACLMO(25) CThreEgAABAOp=A2Op=val
SAACLMO(26) EgAOp=Type=S/SD ---> 1/2
SAACLMO(27) EgAOp=ActiveSpace=Small/Large ---> 2/1
SAACLMO(28) EgAOp=Selection/NoSelection ---> 2/1
SAACLMO(29) EgBOp=Type=S/SD ---> 1/2
SAACLMO(30) EgBOp=ActiveSpace=Small/Large ---> 2/1
SAACLMO(31) EgBOp=Selection/NoSelection ---> 2/1
SAACLMO(32) Ideriv (This is not a keyword)
SAACLMO(33) CThreULS2G=val
SAACLMO(34) CThreULS2E=val
SAACLMO(35) CThreULR1=val
SAACLMO(36) CThreULR2=val
SAACLMO(37) CThreDensULS2=val
SAACLMO(38) CThreDensULR1=val
SAACLMO(39) RefCISD
SAACLMO(40) Flag of keywords
SAACLMO(41) WithoutDegeneracy
SAACLMO(42) EThreDegFac
SAACLMO(43) CThreDegULFac
SAACLMO(44) not used
SAACLMO(45) not used
SAACLMO(46) not used
SAACLMO(47) not used
SAACLMO(48) not used
SAACLMO(49) not used
SAACLMO(50) not used
SAACLMO(51) not used
SAACLMO(52) not used
SAACLMO(53) not used
SAACLMO(54) not used
SAACLMO(55) not used
SAACLMO(56) not used
SAACLMO(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)  ETThreEgR4  
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)  ETThreS2=val  (Global)  
SACThr(14,1)  ETThreR2=val  
SACThr(15,1)  CThreEgULR=val  
SACThr(16,1)  ETThreEGR=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
SACThr(2,2) Variational/NonVariational
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
SACThr(11,2) LinkedSelection/LinkedSelection=N
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)

<table>
<thead>
<tr>
<th>SACMth</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>SD-R/General-R</td>
<td>1/2</td>
</tr>
<tr>
<td>2</td>
<td>SAConly</td>
<td>1/2</td>
</tr>
<tr>
<td>3</td>
<td>SelectionOnly</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>InCoreDiagSAC</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>NonHF</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>PrintMyIOp</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>SkipSmallCI/SmallCI</td>
<td>1/2</td>
</tr>
<tr>
<td>8</td>
<td>not used</td>
<td></td>
</tr>
</tbody>
</table>

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 #ERoute# of L1.F.

(2) MacroIteration: L1.F is modified to make a route for carrying 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 also 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 g01/tests/com.

<table>
<thead>
<tr>
<th>Input No.</th>
<th>SD-R / G-R</th>
<th>Ene. / Opt.</th>
<th>NV / V</th>
<th>Diag.</th>
<th>Molecule</th>
<th>Level</th>
<th>CPU (sec)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>631</td>
<td>SD-R Ene.</td>
<td>NV Iter.</td>
<td>H₂O</td>
<td>N</td>
<td>25s</td>
<td></td>
<td></td>
<td>Singlet, triplet, cation, anion, DZ basis, without selection, comparison with full-CI.</td>
</tr>
<tr>
<td>632</td>
<td>SD-R Ene. V</td>
<td>Iter. H₂O</td>
<td>3</td>
<td>1m33s</td>
<td>Valence-Rydberg singlet &amp; triplet excited states, ionized states compared with experiments.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>633</td>
<td>SD-R Ene. V</td>
<td>Iter. C₂H₄</td>
<td>3,2,1</td>
<td>2m13s</td>
<td>Introductory use of SAC-CI, Nature of the states and SAC-CI dimensions are examined beforehand using SelectCISonly, and then SAC-CI is executed.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>634</td>
<td>SD-R Ene. V</td>
<td>Iter. C₂H₄</td>
<td>3</td>
<td>9m1s</td>
<td>Singlet, triplet, ionized states are compared with exptl. values.</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>635</td>
<td>SD-R Ene. V</td>
<td>Iter. C₂H₄</td>
<td>3,2,1</td>
<td>17m16s</td>
<td>Level1/Level2/Level3 are compared for singlet, triplet, ionized states.</td>
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<tr>
<td>636</td>
<td>SD-R Ene. V</td>
<td>Iter. CO₂</td>
<td>3,2,1</td>
<td>28m32s</td>
<td>Singlet, triplet, ionized, electron-attached states Comparison of Level1/Level 2/Level3 and with exptl.</td>
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<tr>
<td>637</td>
<td>SD-R Ene. V</td>
<td>Iter. Porphin</td>
<td>1</td>
<td>2h43m5s</td>
<td>Free Base Porphin; Q, B, N, L, M bands are calculated with 220 active space.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>638</td>
<td>SD-R Opt. V</td>
<td>Iter. HCF</td>
<td>3</td>
<td>20m31s</td>
<td>Geometry opt of ground A¹ and excited A¹ states and adiabatic excitation energy.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>639</td>
<td>SD-R Opt. V</td>
<td>Iter. NH₂</td>
<td>3</td>
<td>1m24s</td>
<td>Open-shell opt; ground B₁, excited A₁ states are optimized and adiabatic ex. energy calculated.</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>640</td>
<td>SD-R Ene. V</td>
<td>Iter. MoS₄²⁻</td>
<td>2</td>
<td>35m24s</td>
<td>Transition metal complex, On/off of Without-Degeneracy option. Singlet</td>
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<tr>
<td>641</td>
<td>SD-R</td>
<td>Ene.</td>
<td>V</td>
<td>Iter.</td>
<td>Glyoxal</td>
<td>2</td>
<td>24m2s</td>
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<td>642</td>
<td>SD-R</td>
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<td>V</td>
<td>Iter.</td>
<td>Acrolein</td>
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<tr>
<td>643</td>
<td>SD-R</td>
<td>Ene.</td>
<td>NV</td>
<td>InCore</td>
<td>CH$_2$, CH$^+$</td>
<td>F</td>
<td>19m47s</td>
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<tr>
<td>644</td>
<td>SD-R</td>
<td>GSUM</td>
<td>V</td>
<td>InCore</td>
<td>Li$_2$</td>
<td>3</td>
<td>2m33s</td>
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<tr>
<td>645</td>
<td>SD-R</td>
<td>Ene.</td>
<td>V</td>
<td>Iter.</td>
<td>N$_2$</td>
<td>N</td>
<td>5m54s</td>
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<tr>
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<td>Ene.</td>
<td>V</td>
<td>Iter.</td>
<td>N$_2$</td>
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<td>5m37s</td>
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<tr>
<td>647</td>
<td>G-R</td>
<td>Opt.</td>
<td>V</td>
<td>Iter.</td>
<td>BH</td>
<td>3</td>
<td>52s</td>
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<tr>
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<td>V</td>
<td>Iter.</td>
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<td>V</td>
<td>Iter.</td>
<td>HNO</td>
<td>3</td>
<td>1m50s</td>
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<td>Iter.</td>
<td>HCHO</td>
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<td>12m58s</td>
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<tr>
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<td>Opt.</td>
<td>V</td>
<td>Iter.</td>
<td>HCHO</td>
<td>3</td>
<td>25m13s</td>
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<tr>
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<td>Ene.</td>
<td>V</td>
<td>Iter.</td>
<td>CH$_3$, H$_2$O$^+$, NH$_2$</td>
<td>3</td>
<td>7s</td>
<td></td>
</tr>
</tbody>
</table>

Excited states compared with exptl. Singlet, triplet, ionized states are calculated and compared with exptl. 

LMO(Pipek-Mezey) for ground and singlet $n \rightarrow \Pi^*$ excited states, electron correlations are effectively calculated by using LMO. Full linked and unlinked terms within SD-R. Unimportance of the neglected terms. Equivalence of EOM-CC and CCLRT to SAC-CI. 

GSUM: Potential energy curves of 5 singlet states are calculated by the GSUM method. High-spin states (quartet, quintet, sextet, septet), comparison with full-CI. Singlet to septet states by general-R method: results are compared with full-CI. 

General-R opt. Singlet $\Delta$ state (two-electron process; 2ep) is optimized by general-R method giving good agreement with experiment. High-spin opt. Quartet $\Sigma_u^+$ (2ep) and $\Sigma_u^-$ (3ep) are optimized by DT-R and DTQ-R, the latter giving good agreement with experiment. Force at vertical excited state; singlet A', triplet A', ionized A' states; force along internal coordinate. 

All properties (multipole moments, N-th moments, electrostatic properties, diamagnetic terms) Ground (C$_2$), singlet A', triplet A' excited states (C$_2$) are optimized. ESR HFSC, open-shell radicals, full-active.
Electron repulsion integrals are separately allocated in memory and disk.

=== Inputs for detailed program check ===

Comparison of four jobs, NV/V, Iter./InCore
Singlet $\Sigma^-$ state.

Comparison of four jobs, NV/V, Iter./InCore
Triplet $\Pi$ state.

Comparison of four jobs, NV/V, Iter./InCore
Ionized $\Sigma^+$ state.

Comparison of four jobs, NV/V, Iter./InCore
Ionized $\Sigma^+$ state
Electron-attached $\Pi$ state.

Comparison of Canonical and MOD; NV/V, Can.(CMO)/MOD(CMO), singlet $A'$ state.
Combination of GSUM + Opt.
Partial Opt. of H-C-N angle, singlet $A$ excited.

Singlet $\Sigma^-$ state
SDTQ-R.

Open-shell, 2-nd doublet $\Sigma^-$ state of CH by general-R.

Triplet $\Sigma^-$ state of BH, test of SDT-R and SDTQ-R.

Singlet $A'$ state $(C_2)$ is optimized using LMO(PM) by general-R.

Ionized states are calculated with CISD reference.
2ep is obtained by SD-R.

Test of TransitionFrom, ionized, 2-nd state of $A_1$.

Test of TransitionFrom, singlet, 2-nd state of $A_1$.

Satellite peaks, SDTQ-R, FullRGeneration.

Test of TransitionFrom, singlet, 2-nd state of $A_1$.
CH$_3^+$ by SAC, CH$_3$ by electron-attachment of SAC-CI.
CH$_3$ by SAC, triplet state
### Input 631 ###

<table>
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<th>671</th>
<th>SD-R</th>
<th>Ene.</th>
<th>V Iter.</th>
<th>CH₃</th>
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with ROHF MOs.
CH₃ by SAC, CH₃ by ionization of SAC-CI with ROHF MOs.

<table>
<thead>
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<th>3</th>
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CH₃ by SAC, CH₃ by ionization of SAC-CI with ROHF MOs.

<table>
<thead>
<tr>
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<th>G-R</th>
<th>Ene.</th>
<th>V Iter.</th>
<th>H₂O</th>
<th>3</th>
<th>9s</th>
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H₂O⁺⁺ by SAC, H₂O⁺ by electron-attachment of SAC-CI with ROHF MOs of H₂O⁺².

<table>
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<th>G-R</th>
<th>Ene.</th>
<th>V Iter.</th>
<th>H₂O</th>
<th>3</th>
<th>7s</th>
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H₂O by SAC, H₂O⁺ by ionization of SAC-CI with ROHF MOs of H₂O⁺.

<table>
<thead>
<tr>
<th>675</th>
<th>G-R</th>
<th>Ene.</th>
<th>V Iter.</th>
<th>H₂O</th>
<th>3</th>
<th>7s</th>
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</thead>
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<td></td>
</tr>
</tbody>
</table>

H₂O by SAC, H₂O⁺ by ionization of SAC-CI with ROHF MOs of H₂O⁺.

---

* N and F in Level column indicate No selection and No selection with Full-unlinked, respectively.
* CPU time is due to Compaq DS20E

---

**B. Detailed Input Examples**

SAC-CI input examples are given in $g03root/tests/com/test631.com-test675.com. In this guide, test631, test635, test637, test 638, and test647 are shown.

### Input 631 ###

```plaintext
%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);
### 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.
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=(2,3,1,2,2,2,5)),
   Triplet=(NState=(2,3,1,2,2,2,5)),
   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)),

```
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
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<td>.55217497</td>
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</tbody>
</table>
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

Gaussian Test Job 638 (Part 2):
Geometry optimization of the SAC ground state of HCF. Initial geometry is the experimental one. MacroIter=1 (default).
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
game 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 $g03root/tests/sgi/test631.log-test675.log.
In this guide, test631, test635, test637, test 638, and test647 are shown.

### Output 631 ###

Entering Gaussian System, Link 0=/disk0/g03/g03/g03
Initial command:
/disk0/g03/g03/l1.exe /work/g03/inputs/Gau-59185.inp -scrdir=/work/g03/inputs/
Entering Link 1 = /disk0/g03/g03/l1.exe PID= 59186.

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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,

*********************************************
Gaussian 03:   DEC-AXP-OSF/1-G03RevB.01 3-Mar-2003
               1-Apr-2003
*********************************************

%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).

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:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>1</td>
<td>8</td>
<td>0</td>
<td>O</td>
<td>0.000000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>H</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

Distance matrix (angstroms):

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>O</td>
<td>0.000000</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>H</td>
<td>0.975512</td>
<td>0.000000</td>
</tr>
<tr>
<td>3</td>
<td>H</td>
<td>0.975512</td>
<td>1.603685</td>
</tr>
</tbody>
</table>

Stoichiometry: H2O
Framework group: C2V[C2(O),SGV(H2)]
Deg. of freedom: 2
Full point group: C2V NOp 4
Largest Abelian subgroup: C2 NOp 2
Largest concise Abelian subgroup: C2 NOp 2

Standard orientation:

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.
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:


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

Singles-Doubles (SD) SAC/SAC-CI  (SAC-CI SD-R)
STEP #PRES#  Generation of Linked Operators and Selection

== States to be calculated ==

<table>
<thead>
<tr>
<th></th>
<th>A1</th>
<th>A2</th>
<th>B1</th>
<th>B2</th>
</tr>
</thead>
<tbody>
<tr>
<td>SINGLET</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>TRIPLET</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>IONIZED</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>ANIONIZED</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
</tbody>
</table>

== Input data for perturbation selection ==

**SINGLET STATE**

- Number of States Singlet \(= (3, 2, 2, 2)\)
- Main reference configuration \(\text{CThreMainConfig} = 0.100D+00\) (ISEL=2)
- Threshold for perturbation selection of linked operator
  - \(\text{EThreS2 (Lambda_G)} = 0.000D+00\) (au)
  - \(\text{EThreR2 (Lambda_E)} = 0.000D+00\) (au)

**TRIPLET STATE**

- Number of States Triplet \(= (2, 2, 2, 2)\)
- Main reference configuration \(\text{CThreMainConfig} = 0.100D+00\) (ISEL=2)
- Threshold for perturbation selection of linked operator
  - \(\text{EThreR2 (Lambda_E)} = 0.000D+00\) (au)

**IONIZED STATE**

- Number of States CationDoublet \(= (3, 0, 1, 1)\)
- Main reference configuration \(\text{CThreMainConfig} = 0.100D+00\) (ISEL=2)
- Threshold for perturbation selection of linked operator
  - \(\text{EThreR2 (Lambda_E)} = 0.000D+00\) (au)

**ANION STATE**

- Number of States AnionDoublet \(= (2, 0, 1, 2)\)
- Main reference configuration \(\text{CThreMainConfig} = 0.100D+00\) (ISEL=2)
- Threshold for perturbation selection of linked operator
  - \(\text{EThreR2 (Lambda_E)} = 0.000D+00\) (au)

**SINGLET STATE**

- Linked operators for SAC: SYMMETRY = A1 GROUND STATE

<table>
<thead>
<tr>
<th>SELECTION</th>
<th>SINGLE</th>
<th>DOUBLE</th>
<th>TOTAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>BEFORE</td>
<td>19</td>
<td>341</td>
<td>360</td>
</tr>
<tr>
<td>AFTER</td>
<td>19</td>
<td>341</td>
<td>361</td>
</tr>
</tbody>
</table>

- Linked operators for SAC-CI: SYMMETRY = A1 EXCITED STATE

**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
```

<table>
<thead>
<tr>
<th>SELECTION</th>
<th>SINGLE</th>
<th>DOUBLE</th>
<th>TOTAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>BEFORE</td>
<td>19</td>
<td>341</td>
<td>360</td>
</tr>
<tr>
<td>AFTER</td>
<td>19</td>
<td>341</td>
<td>361</td>
</tr>
</tbody>
</table>
LINKED OPERATORS FOR SAC-CI: SYMMETRY = A2  EXCITED STATE
#SECl# 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) = 1.010144
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
#SECl# 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
#SECl# 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
#SECl# Main reference configuration and coefficient
## 1-st state ##  energy (au) = 0.369139
4 -> 6 0.97263 3 -> 7 0.14860
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

II
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

<table>
<thead>
<tr>
<th>SINGLE</th>
<th>DOUBLE</th>
<th>TOTAL</th>
</tr>
</thead>
<tbody>
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<td>270</td>
</tr>
<tr>
<td>AFTER</td>
<td>4</td>
<td>270</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>SINGLE</th>
<th>DOUBLE</th>
<th>TOTAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>BEFORE</td>
<td>8</td>
<td>286</td>
</tr>
<tr>
<td>AFTER</td>
<td>8</td>
<td>286</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>SINGLE</th>
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<th>TOTAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>BEFORE</td>
<td>14</td>
<td>396</td>
</tr>
<tr>
<td>AFTER</td>
<td>14</td>
<td>396</td>
</tr>
</tbody>
</table>

IONIZED STATE

LINKED OPERATORS FOR SAC-CI: SYMMETRY = A1  EXCITED STATE

#SECI# Main reference configuration and coefficient

## 1-st state ##

- energy (au) = 0.552964
- 4 1.00000

## 2-nd state ##

- energy (au) = 1.345949
- 2 1.00000

## 3-th state ##

- energy (au) = 20.558147
- 1 1.00000

SELECTION

<table>
<thead>
<tr>
<th>SINGLE</th>
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<th>TOTAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>BEFORE</td>
<td>3</td>
<td>79</td>
</tr>
</tbody>
</table>

[III]
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

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 WA VE 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

Hartree-Fock configuration   1.00000
================================================================

STEP #ULINTS#  Unlinked integral for Singlet Excited State (SAC-CI)

[Page]
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
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
### 2-nd ### --- 6th state in this spin multiplicity ---

<p>| | | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Total energy in au =</td>
<td>-75.454280</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Correlation energy in au =</td>
<td>0.555558</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Excitation energy in au =</td>
<td>0.701974 in eV = 19.101697</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

*SINGLE EXCITATION*

<p>| | | | |</p>
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<tr>
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<tbody>
<tr>
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<tr>
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<td>0.14298</td>
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<tr>
<td>3 12</td>
<td>0.03793</td>
<td>4 11</td>
<td>-0.03185</td>
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</table>

*DOUBLE EXCITATION*

<p>| | | | |</p>
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<tr>
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<td>-0.03128</td>
<td>5 12</td>
</tr>
</tbody>
</table>

******************************************************************************

Singlet A2

### 1-st ### --- 2nd state in this spin multiplicity ---

<p>| | | | | | | | | |</p>
<table>
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<tr>
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</thead>
<tbody>
<tr>
<td>Total energy in au =</td>
<td>-75.761966</td>
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<td></td>
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<tr>
<td>Correlation energy in au =</td>
<td>0.247871</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Excitation energy in au =</td>
<td>0.394288 in eV = 10.729122</td>
<td></td>
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<td></td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

*SINGLE EXCITATION*

<p>| | | | |</p>
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<tbody>
<tr>
<td>5 7</td>
<td>0.97160</td>
<td>5 12</td>
<td>-0.10814</td>
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*DOUBLE EXCITATION*

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<tr>
<td>5 7</td>
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<td>-0.14357</td>
<td>5 8</td>
</tr>
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<td>5 7</td>
<td>4 6</td>
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<td>3 12</td>
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<td>2 7</td>
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<tr>
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<td>2 11</td>
<td>-0.03745</td>
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<tr>
<td>5 7</td>
<td>4 11</td>
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### 2-nd ### --- 8th state in this spin multiplicity ---

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<tbody>
<tr>
<td>Total energy in au =</td>
<td>-75.181503</td>
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<tr>
<td>Correlation energy in au =</td>
<td>0.828334</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Excitation energy in au =</td>
<td>0.974751 in eV = 26.524322</td>
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*SINGLE EXCITATION*

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<tbody>
<tr>
<td>5 10</td>
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<td>0.07695</td>
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*DOUBLE EXCITATION*

<p>| | | | |</p>
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</thead>
<tbody>
<tr>
<td>5 7</td>
<td>4 6</td>
<td>-0.12591</td>
<td>5 10</td>
</tr>
<tr>
<td>5 6</td>
<td>4 7</td>
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<td>5 10</td>
<td>2 6</td>
<td>-0.05741</td>
<td>5 10</td>
</tr>
</tbody>
</table>
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   | 9    | 5    | 6    | -0.10486 |
| 5   | 6    | 2    | 6    | -0.09802 |
| 5   | 6    | 3    | 12   | 0.08051  |
| 5   | 6    | 4    | 6    | -0.07158 |
| 5   | 7    | 3    | 11   | 0.03878  |
| 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

| 4   | 7    | -0.98251 |
| 3   | 6    | 0.12904  |
| 4   | 12   | 0.08018  |
| 3   | 11   | -0.03904 |

*DOUBLE EXCITATION

| 5   | 8    | 5    | 6    | -0.08035 |
| 5   | 9    | 5    | 8    | 0.06907  |
| 5   | 9    | 4    | 9    | 0.05643  |
| 5   | 6    | 3    | 10   | -0.04677 |
| 5   | 9    | 2    | 6    | -0.03541 |
| 5   | 10   | 4    | 7    | -0.03396 |
| 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  |
| 3   | 11   | -0.03904 |
*DOUBLE EXCITATION

<table>
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<tr>
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<th>7</th>
<th>4</th>
<th>6</th>
<th>0.14773</th>
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<tr>
<td>4</td>
<td>9</td>
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<td>0.09933</td>
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<td>6</td>
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<td>11</td>
<td>3</td>
<td>7</td>
<td>0.03444</td>
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<td>-0.03387</td>
<td>4</td>
<td>12</td>
<td>4</td>
<td>6</td>
<td>-0.03043</td>
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</tbody>
</table>

### 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 = 15.991176

*SINGLE EXCITATION

<table>
<thead>
<tr>
<th>3</th>
<th>6</th>
<th>0.97067</th>
<th>4</th>
<th>7</th>
<th>0.12820</th>
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<tbody>
<tr>
<td>3</td>
<td>9</td>
<td>0.05352</td>
<td>4</td>
<td>10</td>
<td>0.03515</td>
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*DOUBLE EXCITATION

<table>
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<tr>
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<th>7</th>
<th>3</th>
<th>6</th>
<th>-0.15790</th>
<th>4</th>
<th>7</th>
<th>3</th>
<th>7</th>
<th>-0.08071</th>
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<tbody>
<tr>
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<td>10</td>
<td>3</td>
<td>6</td>
<td>-0.05351</td>
<td>4</td>
<td>9</td>
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<td>6</td>
<td>0.04380</td>
</tr>
<tr>
<td>3</td>
<td>12</td>
<td>3</td>
<td>6</td>
<td>0.04330</td>
<td>4</td>
<td>12</td>
<td>2</td>
<td>6</td>
<td>0.04067</td>
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<td>-0.03122</td>
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</tbody>
</table>

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

---

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Solution Excitation energy (eV)</th>
<th>Transition dipole moment (au)</th>
<th>Osc. strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>0</td>
<td>0.0</td>
<td>Excitations are from this state.</td>
</tr>
<tr>
<td>A1</td>
<td>1</td>
<td>10.7545</td>
<td>0.0000</td>
</tr>
<tr>
<td>A1</td>
<td>2</td>
<td>19.1017</td>
<td>0.0000</td>
</tr>
<tr>
<td>A2</td>
<td>1</td>
<td>10.7291</td>
<td>0.0000</td>
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<tr>
<td>A2</td>
<td>2</td>
<td>26.5243</td>
<td>0.0000</td>
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<td>B1</td>
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<td>0.2738</td>
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<tr>
<td>B1</td>
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<td>24.9801</td>
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<tr>
<td>B2</td>
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<td>13.2224</td>
<td>0.0000</td>
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<tr>
<td>B2</td>
<td>2</td>
<td>15.9912</td>
<td>0.0000</td>
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</tbody>
</table>

---

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 spin multiplicity ---
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

### 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
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

---
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<th>in au =</th>
<th>in eV =</th>
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<td>26.091362</td>
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**SINGLE EXCITATION**

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<th>Energy</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 10</td>
<td>0.71791</td>
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<td>5 12</td>
<td>-0.09881</td>
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<tr>
<td>3 8</td>
<td>0.06479</td>
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<td>5 7</td>
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**DOUBLE EXCITATION**

<table>
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<th>Value</th>
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<tbody>
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<td>0.43255</td>
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<td>5 6 4 7</td>
<td>0.31909</td>
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<td>5 7 4 6</td>
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</tr>
<tr>
<td>5 12 3 7</td>
<td>0.11049</td>
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<tr>
<td>5 6 4 12</td>
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<tr>
<td>5 10 5 8</td>
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<td>5 10 4 9</td>
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<td>3 10 5 7</td>
<td>0.05544</td>
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<td>4 10 5 9</td>
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<td>5 7 2 6</td>
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<tr>
<td>5 6 4 10</td>
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<td>4 12 5 6</td>
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<tr>
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<td>2 8 7 11</td>
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**Triplet**

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<tbody>
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<td>3 12</td>
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**SINGLE EXCITATION**

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<td>5 7 4 7</td>
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<tr>
<td>2 11 5 6</td>
<td>-0.03789</td>
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**DOUBLE EXCITATION**

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<th>Value</th>
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<td>5 11</td>
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<td>5 13</td>
<td>0.03089</td>
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**SINGLE EXCITATION**

<table>
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<th>Value</th>
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<tr>
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<tr>
<td>5 9 3 7</td>
<td>0.03248</td>
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---

### 1-st ###

--- 4th state in this spin multiplicity ---

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Total energy in au = -75.722134</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Correlation energy in au = 0.287703</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Excitation energy in au = 0.434120, in eV = 11.813011</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*SINGLE EXCITATION*

| 4 7 | 0.94571 |
| 4 12 | -0.13599 |

*DOUBLE EXCITATION*

| 4 9 4 7 | -0.09520 |
| 3 12 4 7 | 0.06944 |
| 5 8 4 7 | -0.05650 |
| 4 6 2 7 | -0.03479 |
| 3 7 3 6 | -0.03165 |
| 4 12 3 7 | 0.03060 |

---

### 2-nd ###

--- 5th state in this spin multiplicity ---

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Total energy in au = -75.634992</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Correlation energy in au = 0.374846</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Excitation energy in au = 0.521263, in eV = 14.184284</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*SINGLE EXCITATION*

| 3 6 | -0.94546 |
| 3 11 | 0.10887 |
| 3 9 | -0.05096 |
| 2 12 | -0.04080 |

*DOUBLE EXCITATION*

| 4 7 3 7 | 0.07655 |
| 4 9 3 6 | 0.05616 |
| 4 12 2 6 | -0.03730 |
| 3 11 3 7 | -0.03639 |
| 2 13 3 6 | 0.03426 |

---

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

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Solution Excitation energy (eV)</th>
<th>Transition dipole moment (au)</th>
<th>Osc. strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>1.9287</td>
<td>0.1410</td>
<td>0.0000</td>
</tr>
<tr>
<td>A1</td>
<td>8.1972</td>
<td>-0.0202</td>
<td>0.0000</td>
</tr>
</tbody>
</table>
Excitations are from this state.

---

**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 =     34.544709
*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
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 #STATEI#  Monopole Intensity Calculation

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>State</th>
<th>I.P.</th>
<th>Intensity</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>1</td>
<td>13.409</td>
<td>0.95392</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>34.545</td>
<td>0.18681</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>39.133</td>
<td>0.11180</td>
</tr>
<tr>
<td>B1</td>
<td>1</td>
<td>11.632</td>
<td>0.95026</td>
</tr>
<tr>
<td>B2</td>
<td>1</td>
<td>18.824</td>
<td>0.96779</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Solution Energy (eV)</th>
<th>Transition dipole moment (au)</th>
<th>Osc. strength</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>X</td>
<td>Y</td>
</tr>
<tr>
<td>A1</td>
<td>1</td>
<td>1.7771</td>
<td>0.1919</td>
</tr>
<tr>
<td>A1</td>
<td>2</td>
<td>22.9129</td>
<td>-0.2647</td>
</tr>
<tr>
<td>A1</td>
<td>3</td>
<td>27.5008</td>
<td>-0.1943</td>
</tr>
<tr>
<td>B1</td>
<td>1</td>
<td>0.0</td>
<td></td>
</tr>
<tr>
<td>B2</td>
<td>1</td>
<td>7.1924</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

---

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
-- 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 0.03185
3 11 7

### 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 -0.82345 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 0.06403 5 8 9 -0.05427
4 12 7 -0.10742 4 10 7 -0.03913
2 6 6 0.04846 4 11 6 -0.04362
5 6 8 -0.09180 5 8 6 -0.05427
4 7 10 -0.82345 4 12 12 0.03226
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
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

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Solution Excitation energy (eV)</th>
<th>Transition dipole moment (au)</th>
<th>Osc. strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>1 0.0</td>
<td>Excitations are from this state.</td>
<td></td>
</tr>
<tr>
<td>A1</td>
<td>2 17.4348</td>
<td>0.0000 0.0000 -0.7475 0.2387</td>
<td></td>
</tr>
<tr>
<td>B1</td>
<td>1 17.3515</td>
<td>-0.6790 0.0000 0.0000 0.1960</td>
<td></td>
</tr>
<tr>
<td>B2</td>
<td>1 2.4092</td>
<td>0.0000 1.4252 0.0000 0.1199</td>
<td></td>
</tr>
<tr>
<td>B2</td>
<td>2 14.9623</td>
<td>0.0000 1.0397 0.0000 0.3963</td>
<td></td>
</tr>
</tbody>
</table>

Copying SAC-CI densities to excited state density rwf.
0 densities were copied.
Population analysis using the SCF density.

Orbital symmetries:


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  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  YYYX=  -5.5689  ZZZZ=   -6.6383  XXXY=    0.0000
XXXZ=    0.0000  YYYY=    0.0000  YYYY=    0.0000  ZZZX=    0.0000
ZZZY = 0.0000 XXYY = -2.2132 XXZZ = -2.1180 YYYZ = -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-MIRAI85¥SP¥RSACCl¥D95¥H2O1¥MASAHIRO¥01-Apr-2003¥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), ANIONDO UBLET=(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 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, NoUnLinked dSelection). The results are compared with the full-CI results calculated separately. See PartII-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.,-0.5555820926¥H,0,-0.8018426442,0.,-0.5555820926¥¥Version=DEC-A XP-OSF/1-G03RevB.01¥State=1-A¥HF=-76.0098376¥RMSD=5.275e-10¥PG=C02V [ C2(O1),SGV(H2)]¥¥@

ASKING FOR EFFICIENCY AND ADAPTABILITY IN THE SAME PROGRAM IS LIKE ASKING FOR A BEAUTIFUL AND MODEST WIFE ... WE'LL PROBABLY HAVE TO SETTLE FOR ONE OR THE OTHER.

-- THE PSYCHOLOGY OF COMPUTER PROGRAMMING
GERALD M. WEINBERG

Job cpu time: 0 days 0 hours 0 minutes 23.9 seconds.
File lengths (MBytes): RWF= 484 Int= 0 D2E= 0 Chk= 10 Scr= 28

Normal termination of Gaussian 03 at Tue Apr 1 11:23:35 2003.

### Output 635 ###

Entering Gaussian System, Link 0=/disk0/g03/g03/g03
Initial command:
/disk0/g03/g03/l1.exe /work/g03/inputs/Gau-371552.inp -scrdir=/work/g03/inputs/
Entering Link 1 = /disk0/g03/g03/l1.exe PID= 371601.

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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,

# SAC-CI(LevelOne, Singlet=(NState=(2,3,1,2,2,2,5)), Triplet=(NState=
(2,3,1,2,2,2,5)), CationDoublet=(NState=(2,0,1,0,1,1,1))) /Gen Ma
ssage 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.

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

\[
\begin{array}{cccc}
\text{H1} & 1 & r1 \\
\text{C2} & 2 & r2 & 1 \text{ a1} \\
\text{C3} & 3 & r1 & 2 \text{ a1} & 1 & 0 & 0 \\
\text{H4} & 3 & r1 & 2 \text{ a1} & 1 & 180. & 0 \\
\text{H5} & 3 & r1 & 2 \text{ a1} & 1 & 0 & 0 \\
\text{H6} & 2 & r1 & 3 \text{ a1} & 4 & 180. & 0 \\
\text{N7} & 2 & r22 & 1 \text{ a1} & 4 & 0. & 0
\end{array}
\]

Variables:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
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<tbody>
<tr>
<td>r1</td>
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<td>r2</td>
<td>1.3391</td>
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<td>a1</td>
<td>121.28</td>
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<tr>
<td>r22</td>
<td>0.66955</td>
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Input orientation:

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<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
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Distance matrix (angstroms):

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</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
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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)
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
N B a s i s =     6 8  N A E =      8  N B E =      8  N F C =      2  N F V =      0
NROrb=     66 NOA=     6 NOB=     6 NV A=    60 NVB=    60
Semi-Direct transformation.
ModeAB=           4  MOrb=            66 LenV=       5959319
LASXX=       324236 LTotXX=      324236 LenRXX=      324236
LTotAB= 0 MaxLAS=     2679732 LenRXY= 0
NonZer= 648472 LenScr= 1570816 LnRSAI= 5279472
LnScr1= 9424896 LExtra= 0 Total= 16599420
MaxDsk=  -1 SrtSym= T ITran= 5
JobTyp=0 Pass 1:  I= 1 to 66.
(rs|ai) integrals will be sorted in core.

### 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 ==

<table>
<thead>
<tr>
<th>States</th>
<th>AG</th>
<th>B1G</th>
<th>B2G</th>
<th>B3G</th>
<th>AU</th>
<th>B1U</th>
<th>B2U</th>
<th>B3U</th>
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<tbody>
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<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
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<td>TRIPLET</td>
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<td>No</td>
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</table>

---

== Input data for perturbation selection ==

**SINGLET STATE**

Number of States  
Singlet  = ( 3, 3, 3, 1, 2, 2, 2, 5)

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)

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)

Threshold for perturbation selection of linked operator # LevelOne #

EThreR2 (Lambda_E) = 0.100D-05(au)

---

SINGLET STATE

---

**LINKED OPERATORS FOR SAC:**

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<thead>
<tr>
<th>SELECTION</th>
<th>SINGLE</th>
<th>DOUBLE</th>
<th>TOTAL</th>
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<tbody>
<tr>
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<td>9024</td>
<td>9087</td>
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<tr>
<td>AFTER</td>
<td>63</td>
<td>2763</td>
<td>2827</td>
</tr>
</tbody>
</table>

---

**LINKED OPERATORS FOR SAC-CI:**

| SYMMETRY = AG  
| EXCITED STATE |

#SECl# Main reference configuration and coefficient

## 1-st state ##

energy (au) = 0.296334
## 2nd 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
## 1st state ## energy (au) = 0.281843
8 -> 11 0.86335 8 -> 23 0.48630
8 -> 29 0.10227
## 2nd 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
## 3th 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   2845   2874

### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2G EXCITED STATE
#SECI# Main reference configuration and coefficient
## 1st state ## energy (au) = 0.287373
8 -> 10 0.91243 8 -> 24 0.39911
## 2nd 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
## 3th 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
## 1st 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**

<table>
<thead>
<tr>
<th>State</th>
<th>Energy (au)</th>
<th>Selection</th>
</tr>
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<tbody>
<tr>
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<td>27 1341</td>
</tr>
<tr>
<td>2-nd state</td>
<td>0.368854</td>
<td>27 1141</td>
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</table>

### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE

**#SECI# Main reference configuration and coefficient**

<table>
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<th>Energy (au)</th>
<th>Selection</th>
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<tbody>
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<td>0.284181</td>
<td>61 1867</td>
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<tr>
<td>2-nd state</td>
<td>0.331060</td>
<td>61 1928</td>
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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE

**#SECI# Main reference configuration and coefficient**

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<tr>
<th>State</th>
<th>Energy (au)</th>
<th>Selection</th>
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<tbody>
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<td>55 663</td>
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<tr>
<td>2-nd state</td>
<td>0.364234</td>
<td>55 718</td>
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<tr>
<td>3-th state</td>
<td>0.319844</td>
<td>55 718</td>
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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3U EXCITED STATE

**#SECI# Main reference configuration and coefficient**

<table>
<thead>
<tr>
<th>State</th>
<th>Energy (au)</th>
<th>Selection</th>
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<tbody>
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<td>1-st state</td>
<td>0.260350</td>
<td>55 663</td>
</tr>
<tr>
<td>2-nd state</td>
<td>0.315645</td>
<td>55 718</td>
</tr>
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</table>
## 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

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
### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE

**#SECI# Main reference configuration and coefficient**

<table>
<thead>
<tr>
<th>Selection</th>
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<th>Total</th>
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<tbody>
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<tr>
<td>AFTER</td>
<td>35</td>
<td>3447</td>
<td>3482</td>
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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE

**#SECI# Main reference configuration and coefficient**

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<tbody>
<tr>
<td>BEFORE</td>
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<td>12275</td>
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<td>AFTER</td>
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<td>2802</td>
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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = AU EXCITED STATE

**#SECI# Main reference configuration and coefficient**

<table>
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<tr>
<th>Selection</th>
<th>Single</th>
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<th>Total</th>
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<tbody>
<tr>
<td>BEFORE</td>
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<td>10506</td>
<td>10533</td>
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<tr>
<td>AFTER</td>
<td>27</td>
<td>1261</td>
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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE

**#SECI# Main reference configuration and coefficient**

<table>
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<th>Selection</th>
<th>Single</th>
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<th>Total</th>
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<tr>
<td>AFTER</td>
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<td>1873</td>
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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE

**#SECI# Main reference configuration and coefficient**

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<th>Selection</th>
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<th>Double</th>
<th>Total</th>
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<tbody>
<tr>
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<tr>
<td>AFTER</td>
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<td>763</td>
<td>818</td>
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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3U EXCITED STATE

**#SECI# Main reference configuration and coefficient**

<table>
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<th>State</th>
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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = AG EXCITED STATE

**#SECI# Main reference configuration and coefficient**

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<th>Coefficients</th>
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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE

**#SECI# Main reference configuration and coefficient**

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### 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
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

| 8 27 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

===================================================================

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 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 |
| 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 |
### 3-rd ###

--- 14th state in this spin multiplicity ---

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*DOUBLE EXCITATION*

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###   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*

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###   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 |
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 33 0.04874

*DOUBLE EXCITATION
8 25 8 12 -0.08731
8 12 7 33 -0.06997
8 12 6 32 -0.06227
8 12 5 23 -0.05595
8 12 7 37 0.03587
8 35 8 22 0.03673
8 12 4 24 -0.03456
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 33 0.11009

*DOUBLE EXCITATION
8 25 8 22 -0.08269
8 22 7 33 -0.06677
8 22 6 32 -0.06033
8 22 5 23 -0.05275
8 25 8 12 0.04371
8 27 8 23 0.04069
8 22 7 22 -0.03648
8 22 4 24 -0.03312
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  0.04981  8  15  7  22  -0.03501
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

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*******************************************************************************

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**

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**DOUBLE EXCITATION**

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*** 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**

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**DOUBLE EXCITATION**

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*** 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 -0.30427 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 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
### 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

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<th>Solution Excitation energy (eV)</th>
<th>Transition dipole moment (au)</th>
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</table>

### Solution of SDCI

Threshold for density convergence (DConvDiag) 0.100D-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

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<td>Excitation energy in au =</td>
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<tr>
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</table>


**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 |
| 5 | 27 | 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 = 8.511211

**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 | 0.07052 |

**DOUBLE EXCITATION**

|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 8 | 25 | 8 | 23 | -0.07164 | 8 | 35 | 8 | 23 | 0.06820 |
7  8  23 -0.05632  8  25  8  11  0.05200
5  11  0.04864  8  35  8  11 -0.04831
4  8  23  0.04277  5  29  8  23 -0.04158
7  11  0.04128  5  29  8  11  0.03931
6  23  -0.03883  5  34  8  23  0.03793
6  11  0.03729  4  31  8  11 -0.03519
7  23  0.03490  8  33  8  27 -0.03244
8  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 =       7.767718

*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   -0.05268
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   27 -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**

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<th>8 24</th>
<th>-0.07474</th>
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******************************************************************************

**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**

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**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

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### 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 = 10.122828

*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  0.03524
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
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  0.03517  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
### 2-nd state in this spin multiplicity ---

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Total energy in au = -77.945239
Correlation energy in au = 0.105633
Excitation energy in au = 0.367555

### 2-nd state in this spin multiplicity ---

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### 2-nd state in this spin multiplicity ---

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Correlation energy in au = 0.059577
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### 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

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### 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

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### 5-th ###
--- 15th state in this spin multiplicity ---

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Correlation energy in au = 0.100443
Excitation energy in au = 0.362366 in eV = 9.860472

*SINGLE EXCITATION*

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**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)

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Transition dipole moment of triplet state from symmetry B1U 1-th state

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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    -0.09523    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


### 2-nd ### --- 6th state in this spin multiplicity ---

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Total energy in au = -77.422325
Correlation energy in au = 0.628547
Excitation energy in au = 0.890470 in eV = 24.230922

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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
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
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8 17 3  -0.03053  7 46 6  0.03001

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CationDoublet B3G
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<td>5</td>
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<td>5</td>
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<tr>
<td>8</td>
<td>17</td>
<td>3</td>
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<td>7</td>
<td>46</td>
<td>6</td>
<td>0.03001</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*SINGLE EXCITATION
7  0.96508

*DOUBLE EXCITATION
8 27 5  -0.13740  8 18 5  0.09442
<table>
<thead>
<tr>
<th>CationDoublet B1U</th>
<th>1-st</th>
<th>5th state in this spin multiplicity ---</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total energy</td>
<td>-77.600774 au</td>
<td></td>
</tr>
<tr>
<td>Correlation energy</td>
<td>0.450098 au</td>
<td></td>
</tr>
<tr>
<td>Excitation energy</td>
<td>0.712020 au, 19.375057 eV</td>
<td></td>
</tr>
</tbody>
</table>

*SINGLE EXCITATION

| 4 | 0.92236 |

*DOUBLE EXCITATION

| 8 | 27   | 6    | -0.22722 |
| 8 | 27   | 3    | -0.12369 |
| 8 | 36   | 6    | -0.09122 |
| 8 | 25   | 4    | -0.08508 |
| 7 | 30   | 7    | -0.08378 |
| 8 | 31   | 8    | 0.07769 |
| 6 | 18   | 8    | 0.06805 |
| 5 | 28   | 7    | -0.06243 |
| 3 | 27   | 8    | -0.06101 |
| 7 | 43   | 7    | 0.05450 |
| 6 | 41   | 7    | -0.04192 |
| 8 | 45   | 4    | 0.03903 |
| 7 | 41   | 6    | -0.03828 |
| 5 | 42   | 7    | -0.03792 |
| 6 | 26   | 4    | -0.03766 |
| 4 | 24   | 4    | -0.03631 |
| 4 | 31   | 4    | 0.03336 |
| 6 | 36   | 8    | -0.03211 |
| 8 | 38   | 8    | 0.03171 |
| 8 | 47   | 5    | 0.03151 |

<table>
<thead>
<tr>
<th>CationDoublet B2U</th>
<th>4th state in this spin multiplicity ---</th>
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</thead>
<tbody>
<tr>
<td>Total energy</td>
<td>-77.722818 au</td>
</tr>
<tr>
<td>Correlation energy</td>
<td>0.328054 au</td>
</tr>
<tr>
<td>Excitation energy</td>
<td>0.589977 au, 16.054080 eV</td>
</tr>
</tbody>
</table>

*SINGLE EXCITATION

| 5 | 0.94044 |

*DOUBLE EXCITATION

| 8 | 27   | 7    | -0.22980 |
| 8 | 36   | 7    | -0.10093 |
| 8 | 25   | 5    | -0.08697 |
### 1-st state in this spin multiplicity ---

<table>
<thead>
<tr>
<th>Total energy in au</th>
<th>-77.934386</th>
</tr>
</thead>
<tbody>
<tr>
<td>Correlation energy in au</td>
<td>0.116486</td>
</tr>
<tr>
<td>Excitation energy in au</td>
<td>0.378409 in eV = 10.297024</td>
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</tbody>
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**SINGLE EXCITATION**

| 8   | 0.97508 |

**DOUBLE EXCITATION**

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<tr>
<th>8</th>
<th>-0.09809</th>
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<th>35</th>
<th>8</th>
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</thead>
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<td>7</td>
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<td>29</td>
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<tr>
<td>6</td>
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<td>4</td>
<td>31</td>
<td>8</td>
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</tr>
<tr>
<td>5</td>
<td>-0.06231</td>
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<td>34</td>
<td>8</td>
<td>0.05709</td>
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<tr>
<td>7</td>
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</tr>
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<td>17</td>
<td>8</td>
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<tr>
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<td>8</td>
<td>0.03233</td>
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**STEP #SATEI#  Monopole Intensity Calculation**

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<th>State</th>
<th>I.P.</th>
<th>Intensity</th>
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<tr>
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<td>14.569</td>
<td>0.92274</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>24.231</td>
<td>0.72985</td>
</tr>
<tr>
<td>B3G</td>
<td>1</td>
<td>12.882</td>
<td>0.93138</td>
</tr>
<tr>
<td>B1U</td>
<td>1</td>
<td>19.375</td>
<td>0.85074</td>
</tr>
<tr>
<td>B2U</td>
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<td>16.054</td>
<td>0.88443</td>
</tr>
<tr>
<td>B3U</td>
<td>1</td>
<td>10.297</td>
<td>0.95078</td>
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</table>

**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. strength
--- | --- | --- | --- | ---
 | energy (eV) | X | Y | Z |
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)

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):

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<tr>
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<th>4</th>
<th>5</th>
<th>6</th>
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<tbody>
<tr>
<td>C</td>
<td>0.527370</td>
<td>0.412861</td>
<td>-0.038682</td>
<td>-0.005602</td>
<td>0.002285</td>
<td>-0.030002</td>
</tr>
<tr>
<td>C</td>
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<td>4.861946</td>
<td>0.619506</td>
<td>-0.038682</td>
<td>-0.038682</td>
<td>0.412861</td>
</tr>
<tr>
<td>C</td>
<td>-0.038682</td>
<td>0.619506</td>
<td>4.861946</td>
<td>0.412861</td>
<td>0.412861</td>
<td>-0.038682</td>
</tr>
<tr>
<td>H</td>
<td>-0.005602</td>
<td>-0.038682</td>
<td>0.412861</td>
<td>0.527370</td>
<td>-0.030002</td>
<td>0.002285</td>
</tr>
</tbody>
</table>
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

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:

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<tbody>
<tr>
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<td>C</td>
<td>C</td>
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<td>H</td>
<td>H</td>
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</tbody>
</table>

<table>
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<th>4</th>
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<th>7</th>
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</thead>
<tbody>
<tr>
<td>H</td>
<td>C</td>
<td>C</td>
<td>H</td>
<td>H</td>
<td>H</td>
<td>Bq</td>
</tr>
</tbody>
</table>

Sum of Mulliken charges= 0.000000

Atomic charges with hydrogens summed into heavy atoms:

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<th>4</th>
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<th>7</th>
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</thead>
<tbody>
<tr>
<td>H</td>
<td>H</td>
<td>H</td>
<td>H</td>
<td>Bq</td>
<td></td>
<td></td>
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</tbody>
</table>

Sum of Mulliken charges= 0.000000

Electronic spatial extent (au): <R**2>= 83.5302
Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

<table>
<thead>
<tr>
<th>X</th>
<th>Y</th>
<th>Z</th>
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</thead>
<tbody>
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<td>0.0000</td>
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</tbody>
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Quadrupole moment (field-independent basis, Debye-Ang):

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<th>XX</th>
<th>YY</th>
<th>ZZ</th>
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</thead>
<tbody>
<tr>
<td>-16.2640</td>
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<td>-12.1376</td>
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</tbody>
</table>

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

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<th>ZZ</th>
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</thead>
<tbody>
<tr>
<td>-2.7013</td>
<td>1.2763</td>
<td>1.4250</td>
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Octapole moment (field-independent basis, Debye-Ang**2):

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<th>YYY</th>
<th>ZZZ</th>
<th>XYY</th>
<th>YZZ</th>
<th>ZXX</th>
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<tbody>
<tr>
<td>0.0000</td>
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<td>0.0000</td>
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Hexadecapole moment (field-independent basis, Debye-Ang**3):

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<th>XXXY</th>
<th>YYYZ</th>
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<tr>
<td>-21.6535</td>
<td>-27.0739</td>
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<table>
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<tbody>
<tr>
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<table>
<thead>
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<tbody>
<tr>
<td>-8.8502</td>
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<table>
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<tbody>
<tr>
<td>-16.1757</td>
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Test job not archived.

1¥1¥GINC-MIRAI85¥SP¥RSACCI¥Gen¥C2H4N1¥MASAHIRO¥10-May-2003¥¥ SAC-CI (LEVELONE, SINGLET=(NSTATE=(2,3,1,2,2,2,5)), TRIPLET=(NSTATE=(2,3,1,2,2,2,5)), CATIONDOUBLET=(NSTATE=(2,0,0,1,0,1,1,1))) /GEN MASSAGE IO P(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¥H¥C,1,1.0868¥C,2,1.3391,1,121.28¥H,3,1.0868,2,121.28,1,0.,0¥H,3,1.0868,2,121.28,4,180.,0¥H,2,1.0868,3,121.28,4,180.,0¥H,1,0.66955,1,121.28,4,0.,0¥Bq,2,0.66955,1,121.28,4,0.,0¥¥Version=DEC-AXP-OSF/1-G03RevB.01¥¥State=1 AG¥¥HF=-78.050872¥YRMSD=3.635e-09¥YPG=D02H [O(N1),C2"(C1.C1),SG(H4)]¥¥

TERENCE, THIS IS STUPID STUFF:
YOU EAT YOUR VICTUALS FAST ENOUGH;
THERE CAN'T BE MUCH AMISS, 'TIS CLEAR
TO SEE THE RATE YOU DRINK YOUR BEER.
BUT OH, GOOD LORD, THE VERSE YOU MAKE,
IT GIVES A CHAP THE BELLY-ACHE.
THE COW, THE OLD COW, SHE IS DEAD;
IT SLEEPS WELL, THE HORNED HEAD:
WE POOR LADS, 'TIS OUR TURN NOW
TO HEAR SUCH TUNES AS KILLED THE COW.
PRETTY FRIENDSHIP 'TIS TO RHYME
YOUR FRIENDS TO DEATH BEFORE THEIR TIME.
MOPING, MELANCHOLY MAD:
COME PIPE A TUNE TO DANCE TO, LAD.

-- A. E. HOUSMAN
Job cpu time:  0 days  0 hours  3 minutes 16.1 seconds.
File lengths (MBytes):  RWF=    543 Int=      0 D2E=      0 Chk=     13 Scr=     48
Normal termination of Gaussian 03 at Sat May 10 12:24:34 2003.
Initial command:
/disk0/g03/g03/l1.exe /work/g03/inputs/Gau-371552.inp -scrdir=/work/g03/inputs/
Entering Link 1 = /disk0/g03/g03/l1.exe PID= 371594.

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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 03: DEC-AXP-OSF/1-G03RevB.01 3-Mar-2003
10-May-2003

# SAC-CI(LevelTwo, Singlet=(NState=(2,3,1,2,2,2,5)), Triplet=(NState=(2,3,1,2,2,2,5)), CationDoublet=(NState=(2,0,0,1,0,1,1,1))) /Gen Message IOP(2/15=-1) test

1/38=1/1;
2/15=-1,17=6,18=5,40=1/2;
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:

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<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
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<td>0.000000 0.000000 0.000000</td>
</tr>
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<td>6</td>
<td>0</td>
<td>0.000000 0.000000 1.086800</td>
</tr>
<tr>
<td>3</td>
<td>6</td>
<td>0</td>
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Distance matrix (angstroms):

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<th>4</th>
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<tr>
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<td>3</td>
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<tr>
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Gaussian Test Job 635 (Part 2): SAC-CI SD-R LevelTwo calculations for ethylene.
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:

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<th>Atomic Number</th>
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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.

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 33.249942363 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
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
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

Semi-Direct transformation.
ModeAB=           4 MOrb=             66 LenV=  5959319
LASXX=       324236 LTotXX=  324236 LenRXX=  324236
LTotAB=           0 MaxLAS=  2679732 LenRXY=  0
NonZer=       648472 LenScr=  1570816 LnRSAI=  5279472
LnScr1=     9424896 LEextra=  0 Total=  16599420
MaxDsk=      -1 SrtSym=             T ITran=  5
JobTyp=0 Pass 1:  I=  1 to  66.
(rs|ai) integrals will be sorted in core.

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 ==

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<th>B1G</th>
<th>B2G</th>
<th>B3G</th>
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<td>Yes</td>
<td>Yes</td>
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<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
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<td>No</td>
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</table>

== 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
<table>
<thead>
<tr>
<th>SELECTION</th>
<th>SINGLE</th>
<th>DOUBLE</th>
<th>TOTAL</th>
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<tbody>
<tr>
<td>BEFORE</td>
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<td>9024</td>
<td>9087</td>
</tr>
</tbody>
</table>

[III]
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: 63, 9024, 9087
- DOUBLE: 63, 1980, 2044
- TOTAL: 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
- 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: 29, 7364, 7393
- DOUBLE: 29, 3298, 3327
- TOTAL: 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
- 6 -> 27: -0.27427, 6 -> 18: 0.26566
- 8 -> 24: 0.15588
- 8 -> 10: -0.14036, 6 -> 14: -0.10387

**SELECTION**
- SINGLE: 35, 7484, 7519
- DOUBLE: 35, 3309, 3344
- TOTAL: 35, 7484, 7519

---

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
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<td>AFTER</td>
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<td>2545</td>
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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = AU EXCITED STATE

#### #SECI# Main reference configuration and coefficient

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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE

#### #SECI# Main reference configuration and coefficient

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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE

#### #SECI# Main reference configuration and coefficient

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<table>
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<th>3-th state</th>
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</table>
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

T R I P L E T  S T A T E

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
3-th state

**SELECTION**

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**AFTER**

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**LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE**

**#SECI# Main reference configuration and coefficient**

**## 1-st state ##**

| energy (au) | 0.364354 |

**## 2-nd state ##**

| -0.10797 | 0.84635 |

| -0.10124 | 0.11741 |

**SELECTION**

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</table>

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**LINKED OPERATORS FOR SAC-CI: SYMMETRY = AU EXCITED STATE**

**#SECI# Main reference configuration and coefficient**

**## 1-st state ##**

| energy (au) | 0.370044 |

| 0.77647 | 0.44073 |

| -0.21913 | 0.17377 |

| 0.11173 |

| 0.11173 |

| 7 -> 9 | 7 -> 26 |

| 7 -> 19 | 7 -> 28 |

| 5 -> 24 | 5 -> 10 |

| 7 -> 16 |

**SELECTION**

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<tr>
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---

**LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE**

**#SECI# Main reference configuration and coefficient**

**## 1-st state ##**

| energy (au) | 0.129560 |

| 0.71782 | 0.66032 |

| 0.17938 | 0.10220 |

| 0.71782 |

| 0.66032 |

| 0.17938 |

| 0.10220 |

| 8 -> 27 | 8 -> 18 |

| 8 -> 36 | 8 -> 14 |

| 8 -> 27 | 8 -> 27 |

| 8 -> 18 |

**SELECTION**

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**AFTER**

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**LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2U EXCITED STATE**

**#SECI# Main reference configuration and coefficient**

**## 1-st state ##**

| energy (au) | 0.319743 |

| 0.86916 | 0.49394 |

| 0.86916 |

| 0.49394 |

| 0.86916 |

| 0.49394 |

| 0.86916 |

| 0.49394 |

| 8 -> 15 | 8 -> 20 |

| 8 -> 18 |

| 8 -> 27 |

| 8 -> 27 |

| 8 -> 18 |

| 8 -> 27 |

| 8 -> 27 |

| 8 -> 14 |

**SELECTION**

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**AFTER**

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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   0.15679
## 3-th state ##  energy (au) =  0.315979
8 -> 13   0.68319  8 ->  21  0.49465
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

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 1.0000

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 1.0000

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
*SINGLE 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

ENERGY AND WAVE FUNCTION OF SAC-CI METHOD

***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 #SCIIV# 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 = 8.189001
*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

*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
### 3-rd ###           --- 14th state in this spin multiplicity ---

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<th>Energy</th>
<th>Value</th>
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### 1-st ###           --- 3rd state in this spin multiplicity ---

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### 2-nd ###           --- 2nd state in this spin multiplicity ---

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<td>Excitation energy</td>
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### 1-nd ###           --- 1st state in this spin multiplicity ---

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### 0-th ###           --- 0th state in this spin multiplicity ---

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<tr>
<td>Excitation energy</td>
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<td>in eV</td>
<td>7.859047</td>
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</table>
### 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  4  27  -0.07197  
8  25  8  10  0.04129  8  24  5  23  -0.03279  
8  24  7  37  0.03276  8  27  4  18  -0.03193  
8  24  24  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  24  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  
8  38  4  27  -0.03109  8  24  4  27  -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


### 1-st ###           --- 7th state in this spin multiplicity ---

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### 2-nd ###           --- 18th state in this spin multiplicity ---

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### 3-rd ###           --- 4th state in this spin multiplicity ---

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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 = 10.079776

*SINGLE EXCITATION
### 1-st ###
--- 1st state in this spin multiplicity ---

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<td>-78.058092</td>
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<td>0.264353 (7.193408 eV)</td>
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### SINGLE EXCITATION ###
- 8 13: -0.87859
- 8 16: -0.16640
- 8 19: 0.15048
- 8 28: 0.07382
- 8 32: 0.03338

### DOUBLE EXCITATION ###
- 8 25 8 20: 0.08920
- 8 25 8 26: 0.03422
- 8 35 8 9: -0.08152

### 2-nd ###
--- 6th state in this spin multiplicity ---

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<tr>
<td>-77.999995</td>
<td>0.050877</td>
<td>0.322450 (8.774309 eV)</td>
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### SINGLE EXCITATION ###
- 8 13: 0.75116
- 8 16: 0.26877
- 8 21: 0.06343
- 8 32: 0.03338

### DOUBLE EXCITATION ###
- 8 25 8 13: -0.07535
- 8 25 8 19: 0.05055
- 8 35 8 19: -0.03492

### 3-rd ###
--- 8th state in this spin multiplicity ---

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<tr>
<td>-77.999995</td>
<td>0.050877</td>
<td>0.322450 (8.774309 eV)</td>
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</table>

### SINGLE EXCITATION ###
- 8 13: -0.07535
- 8 16: 0.26877
- 8 21: 0.06343
- 8 32: 0.03338

### DOUBLE EXCITATION ###
- 8 25 8 13: -0.07535
- 8 25 8 19: -0.03492
### 4-th Energy Level --- 12th State in This Spin Multiplicity ---

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### Single Excitation

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### 5-th Energy Level --- 15th State in This Spin Multiplicity ---

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### 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

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### CI matrix elements

#### TRIPLET STATE

### Solution of SDCI

Threshold for density convergence (DConvDiag): 0.100D-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
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**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

---

### 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

---

### 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

---

*DOUBLE EXCITATION*
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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 | 9.663526 |

***SINGLE EXCITATION***

| 6 | 18 | -0.67899 |
| 6 | 36 | 0.15889 |
| 8 | 24 | -0.04744 |
| 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 | 10.046212 |

***SINGLE EXCITATION***
*

**Triplet B3G**

--- 12th state in this spin multiplicity ---

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<td>Excitation energy in au =</td>
<td>0.351986 in eV = 9.578035</td>
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**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 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 AU**

--- 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 |
### 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 |

*SINGLE EXCITATION

| 8 27 | 0.69910 | 8 18 | -0.66598 |
| 8 36 | 0.17317 | 8 14 | -0.11200 |

*SINGLE EXCITATION

| 8 25 | 0.92626 | 8 27 | 0.26998 |
| 8 18 | 0.13891 | 8 36 | 0.05091 |

*SINGLE EXCITATION

| 8 27 | 0.69910 | 8 18 | -0.66598 |
| 8 36 | 0.17317 | 8 14 | -0.11200 |

*SINGLE EXCITATION

| 8 25 | 0.92626 | 8 27 | 0.26998 |
| 8 18 | 0.13891 | 8 36 | 0.05091 |
### 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 20 8 15 0.08168 8 35 8 15 -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 0.03693 7 37 8 9 0.03893
5 23 8 9 -0.03793 4 24 8 9 -0.03180
### 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 0.04126
6 32 8 13 -0.05025 4 31 8 13 -0.03516
7 33 8 19 -0.03521 5 23 8 13 -0.03421
8 25 8 16 -0.03427 5 29 8 19 -0.03525
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 -0.03458 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 = 9.675437

*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
### 5-th state in this spin multiplicity ---

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**Total energy** in au = -77.958898

**Correlation energy** in au = 0.091974

**Excitation energy** in au = 0.363547 in eV = 9.892610

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**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**

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<th>Symmetry</th>
<th>Solution Excitation energy (eV)</th>
<th>Transition dipole moment (au)</th>
<th>Osc. strength</th>
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<tr>
<td>B1G</td>
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| 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

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### 2-nd ###  --- 6th state in this spin multiplicity ---

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### SINGLE EXCITATION

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### DOUBLE EXCITATION

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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

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*******************************************************************************
Cation Doublet 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

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STEP #STATEI# 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

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<tr>
<th>Symmetry</th>
<th>Solution Excitation energy (eV)</th>
<th>Transition dipole moment (au)</th>
<th>Osc. strength</th>
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<td>0.1152 0.0000 0.0000</td>
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<td>2 13.9464</td>
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<td>Excitations are from this state.</td>
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---

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)
(B3U) (B2G) (B3G) (B1U) (AG) (B1U) (B2U) (AG)
(B1U) (B1G) (B3U) (B3G) (AG) (B3G) (AG) (B2U)
(B1U) (B2G) (B2U) (B3U) (B1G) (B1U) (B2G) (AG)
(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):

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<td>0.002285</td>
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Mulliken atomic charges:

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Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

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</table>

Sum of Mulliken charges= 0.00000

Electronic spatial extent (au): \( <R^2> = 83.5302 \)

Charge= 0.00000 electrons

Dipole moment (field-independent basis, Debye):

\[
X = 0.0000 \quad Y = 0.0000 \quad Z = 0.0000 \quad \text{Tot} = 0.0000
\]

Quadrupole moment (field-independent basis, Debye-Ang):

\[
XX = -16.2640 \quad YY = -12.2863 \quad ZZ = -12.1376
\]

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

\[
XX = -2.7013 \quad YY = 1.2763 \quad ZZ = 1.4250
\]

Octapole moment (field-independent basis, Debye-Ang**2):

\[
\text{[content not visible here]}
\]
Hexadecapole moment (field-independent basis, Debye-Ang*3):

\[
\begin{align*}
XXX &= -21.6535 & YYY &= -27.0739 & ZZZ &= -68.5119 \\
XXX &= & YYY &= 0.0000 & ZZZ &= 0.0000 \\
ZZZ &= & XXX &= 0.0000 & YYY &= 0.0000 \\
ZZZ &= & XXX &= 0.0000 & YYY &= 0.0000 \\
XYZ &= & XXX &= 0.0000 & YYY &= 0.0000 \\
XYZ &= & XXX &= 0.0000 & YYY &= 0.0000 \\
XYY &= & XXX &= 0.0000 & YYY &= 0.0000 \\
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ZZY &= & XXX &= 0.0000 & YYY &= 0.0000 \\
ZZY &= & XXX &= 0.0000 & YYY &= 0.0000 \\
XZ &= & XXX &= 0.0000 & YYY &= 0.0000 \\
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Z &= & XXX &= 0.0000 & YYY &= 0.0000 \\
}\end{align*}
\]

Test job not archived.

```
1¥1¥GINC-MIRAI8¥SP¥RSACCI¥Gen¥C2H4N1¥MASAHIRO¥10-May-2003¥0¥¥# SAC-CI
(LEVELTWO, SINGLET=(NSTATE=(2,3,1,2,2,2,5)), TRIPLET=(NSTATE=(2,3,3,1,2,2,2)),
CATIONDOUBLET=(NSTATE=(2,0,0,1,0,1,1,1))) /GEN MASSAGE IO
P(2/15=-1) TEST¥¥Gaussian Test Job 635 (Part 2): SAC-CI SD-R LevelTwo
calculations 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.,1,180.,2¥H,2,1.0868,3,121.28
,4,180.,¥Bq,2,0.66955,1,121.28,4,0.,0¥¥Version=DEC-AXP-OSF/1-G03RevB.
01¥State=1-AG¥HF=+78.050872¥RMSD=3.635e-09¥PG=D02H [O(N1),C2"(C1.C1),S
G(H4)]¥¥@
```

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METHODS WHICH THEY USE, I ADVISE YOU TO FOLLOW THIS PRINCIPLE VERY
STRICTLY:
DONT LISTEN TO THEIR WORDS; PAY ATTENTION, INSTEAD, TO THEIR ACTIONS.
-- A.EINSTEIN, 1934

Job cpu time:  0 days  0 hours  4 minutes 49.5 seconds.

Initial command:
/disk0/g03/g03/1.exe /work/g03/inputs/Gau-371552.inp -scrdir=/work/g03/inputs/
Entering Link 1 = /disk0/g03/g03/1.exe PID= 371653.

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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 03: DEC-AXP-OSF/1-G03RevB.01 3-Mar-2003
10-May-2003

# 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=(2,0,1,0,1,1,1))) /Gen
Massage IOP(2/15=-1) 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 3): SAC-CI SD-R LevelThree 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:

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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:
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<th>Coordinates (Angstroms)</th>
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Rotation 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
Semi-Direct transformation.
ModeAB= 4 MOrb= 66 LenV= 5959319
LASXX= 324236 LTotXX= 324236 LenRXX= 324236
LTotAB= 0 MaxLAS= 2679732 LenRXY= 0
NonZer= 648472 LenScr= 1570816 LnRSAI= 5279472
LnScr1= 9424896 LExtra= 0 Total= 16599420
MaxDsk= -1 SrtSym= 5 ITran= 5
JobTyp=0 Pass 1: I= 1 to 66.
(rsai) integrals will be sorted in core.

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  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  =  (3, 2, 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, 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, 1, 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
## 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

#SECI# Main reference configuration and coefficient

<table>
<thead>
<tr>
<th>State</th>
<th>Energy (au)</th>
<th>8 -&gt; 11</th>
<th>8 -&gt; 23</th>
<th>8 -&gt; 29</th>
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<tbody>
<tr>
<td>1-st</td>
<td>0.281843</td>
<td>0.86335</td>
<td>0.48630</td>
<td>0.10227</td>
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<tr>
<td>2-nd</td>
<td>0.341571</td>
<td>0.72120</td>
<td>0.48630</td>
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<tr>
<td>3-th</td>
<td>0.356963</td>
<td>0.82116</td>
<td>0.48630</td>
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**SELECTION**

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<td>AFTER</td>
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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B2G EXCITED STATE

#SECI# Main reference configuration and coefficient

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<tr>
<th>State</th>
<th>Energy (au)</th>
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<th>6 -&gt; 27</th>
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<tr>
<td>1-st</td>
<td>0.287373</td>
<td>0.91243</td>
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<td>2-nd</td>
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<td>3-th</td>
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**SELECTION**

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<td>AFTER</td>
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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE

#SECI# Main reference configuration and coefficient

<table>
<thead>
<tr>
<th>State</th>
<th>Energy (au)</th>
<th>7 -&gt; 9</th>
<th>7 -&gt; 26</th>
<th>7 -&gt; 19</th>
<th>5 -&gt; 24</th>
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<tbody>
<tr>
<td>1-st</td>
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**SELECTION**

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### LINKED OPERATORS FOR SAC-CI: SYMMETRY = AU EXCITED STATE

#SECI# Main reference configuration and coefficient

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<tr>
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<td>0.320962</td>
<td>0.90268</td>
<td>0.42641</td>
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</table>
# 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 0.72792 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
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 ##

<table>
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<td>0.40646</td>
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## 3-th state ##

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<th>Transition</th>
<th>Energy (au)</th>
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## 4-th state ##

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## 5-th state ##

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**LINKED OPERATORS FOR SAC-CI: SYMMETRY = AG EXCITED STATE**

### SECl# Main reference configuration and coefficient

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**IONIZED STATE**

**LINKED OPERATORS FOR SAC-CI: SYMMETRY = B3G EXCITED STATE**

### SECl# Main reference configuration and coefficient

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**LINKED OPERATORS FOR SAC-CI: SYMMETRY = B1U EXCITED STATE**

### SECl# Main reference configuration and coefficient

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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 |
### 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\text{ 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\text{ 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\text{ 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 |
### 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
### 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

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

Singlet  B3G

*******************************************************************************

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  12  -0.08281  8  35  8  12  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 =      8.194772

*SINGLE EXCITATION
  8  18  0.80472  8  14  0.42228  
  8  27 -0.34117  6  38  0.06766  
  7  29 -0.06281  7  33  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
### 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   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

*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

### 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

*SINGLE 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 B3U**

### 1-st ###
--- 1st state in this spin multiplicity ---

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*SINGLE EXCITATION*

8  9  0.87879
8  16 0.16721
8  13 0.07499
8  32 0.03968

*DOUBLE EXCITATION*

8  25  8  9  -0.08920
8  9  7  33  -0.06612
8  9  6  32  -0.05927
8  9  5  34  0.04193
8  26  8  25  -0.03385
8  9  7  22  -0.03101

### 2-nd ###
--- 6th state in this spin multiplicity ---

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*SINGLE EXCITATION*

8  13  0.75158
8  16 0.26869
8  21 0.06365
8  32 0.03339

*DOUBLE EXCITATION*

8  25  8  13  -0.07537
8  13  7  33  -0.05919
8  13  6  32  -0.05408
8  13  4  31  0.05194
8  13  5  23  -0.03759
8  13  7  37  0.03584
8  19  4  31  0.03157
8  19  6  32  -0.03100

### 3-rd ###
--- 8th state in this spin multiplicity ---

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*SINGLE EXCITATION*

8  16  -0.78430
8  13  0.30165
8  19  -0.08201
8  28  -0.03027

*DOUBLE EXCITATION*
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### 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

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*DOUBLE EXCITATION

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### 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

<p>| | | | | | |</p>
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</table>

*DOUBLE EXCITATION

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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

<table>
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<tr>
<th>Symmetry</th>
<th>Solution</th>
<th>Excitation energy (eV)</th>
<th>Transition dipole moment (au)</th>
<th>Osc. strength</th>
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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

### 1-st ###           ---  5th state in this spin multiplicity ---

Total energy in au = -78.038528
Correlation energy in au = 0.012344
Excitation energy in au = 0.296215 in eV = 8.060406

*SINGLE EXCITATION
8 17 0.88401
8 35 -0.06955

*DOUBLE EXCITATION
8 35 8 17 0.08426
7 32 8 17 -0.06155
5 23 8 17 -0.05462
7 37 8 17 0.04803
4 24 8 17 -0.03249

### 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 35 -0.13798

*DOUBLE EXCITATION
8 35 8 25 0.07830
7 33 8 25 -0.06105
5 29 8 25 -0.05533
8 35 8 17 -0.04254
5 25 8 23 0.03727
8 23 5 25 0.03325
6 32 8 17 0.03183

II
### 1-st ###           --- 4th state in this spin multiplicity ---

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<td>Excitation energy in au</td>
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*DDOUBLE EXCITATION*

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<td>8 35</td>
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<td>8 23</td>
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### 2-nd ###           --- 6th state in this spin multiplicity ---

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<tr>
<td>Excitation energy in au</td>
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</table>

*SINGLE EXCITATION*

| 7 18 | 0.70681 |
| 7 14 | 0.13467 |
| 8 11 | 0.07205 |

*DDOUBLE EXCITATION*

<table>
<thead>
<tr>
<th>8 27</th>
<th>5 18</th>
<th>-0.10726</th>
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<tbody>
<tr>
<td>8 27</td>
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<tr>
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### 3-rd ###           --- 15th state in this spin multiplicity ---

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<td>Excitation energy in au</td>
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</table>

*SINGLE EXCITATION*

| 8 23 | 0.81100 |
| 8 29 | 0.21049 |
| 7 18 | 0.04028 |

*DDOUBLE EXCITATION*

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Triplet B2G

### 1-st ### --- 3rd state in this spin multiplicity ---

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</table>

*SINGLE EXCITATION*

| 8 10 | 0.86151 |
| 8 24 | 0.43761 |
| 8 31 | -0.12222 |

*DOUBLE EXCITATION*

| 8 25 | 8 10 | -0.08318 |
| 7 33 | 8 10 | -0.06779 |
| 6 32 | 8 10 | -0.06214 |
| 5 23 | 8 10 | -0.05239 |
| 5 34 | 8 10 | 0.04097 |
| 8 27 | 8 26 | 0.03997 |
| 8 35 | 8 24 | 0.03613 |
| 7 22 | 8 10 | -0.03046 |

### 2-nd ### --- 13th state in this spin multiplicity ---

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*SINGLE EXCITATION*

| 6 18 | -0.67722 |
| 6 36 | 0.15921 |
| 8 24 | -0.05011 |
| 8 10 | 0.04635 |

*DOUBLE EXCITATION*

| 8 27 | 4 18 | 0.07532 |
| 8 18 | 4 27 | 0.05480 |
| 8 35 | 6 18 | -0.03314 |
| 8 35 | 6 36 | -0.03200 |
| 8 25 | 8 10 | 0.04897 |
| 8 35 | 8 10 | -0.04548 |
| 4 31 | 8 24 | 0.04363 |
| 7 22 | 8 10 | -0.03046 |

### 3-rd ### --- 18th state in this spin multiplicity ---

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*SINGLE EXCITATION*

| 8 24 | 0.82924 |
| 8 31 | -0.21917 |
| 8 40 | 0.04756 |
| 8 30 | -0.04118 |

*DOUBLE EXCITATION*

| 8 25 | 8 24 | -0.07444 |
| 5 29 | 8 24 | -0.06038 |
| 7 33 | 8 24 | -0.05537 |
| 8 25 | 8 10 | 0.04897 |
| 4 31 | 8 24 | 0.04363 |
| 8 24 | 5 23 | 0.03743 |
| 6 32 | 8 10 | 0.03580 |
### 1-st ###           ---  12th state in this spin multiplicity ---

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### 2-nd ###           ---  19th state in this spin multiplicity ---

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*necessary corrections*

**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

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### 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

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### 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

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### 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

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Triplet B3U

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--- 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

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--- 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

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III
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Total energy in au = -78.007237  
Correlation energy in au = 0.043635  
Excitation energy in au = 0.327505  in eV = 8.911872

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*DOUBLE EXCITATION

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*SINGLE EXCITATION

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### 5-th ###  --- 16th state in this spin multiplicity ---

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STEP #DENS#  Density Calculation

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

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<th>Solution Excitation energy (eV)</th>
<th>Transition dipole moment (au)</th>
<th>Osc. strength</th>
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STEP #CIMX#  CI matrix elements

### IONIZED STATE ###

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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 ---
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Correlation energy in au = 0.611332
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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 |

*DOUBLE EXCITATION

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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  27  3  -0.12307  
6  27  8  -0.09084  
8  25  4  -0.08515  
7  30  7  -0.08358  
6  29  7  0.07771  
6  18  8  0.06620  
5  28  7  -0.06233  
3  27  8  -0.06120  
7  43  7  0.05460  
6  41  7  -0.04125  
8  45  4  0.03842  
5  42  7  -0.03789  
7  42  5  -0.03780  
6  26  4  -0.03657  
4  24  4  -0.03542  
4  31  4  0.03293  
6  36  8  -0.03140  
8  47  5  0.03127  
8  38  8  0.03122

*******************************************************************************

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  36  7  -0.10009  
8  25  5  -0.08710  
7  33  5  -0.06455  
5  23  5  -0.05197  
6  38  7  -0.04215  
5  34  5  0.03892  
6  32  5  -0.03568  
4  31  5  0.03316  
7  36  8  -0.03069

*******************************************************************************

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

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STEP #SATEI# Monopole Intensity Calculation

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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

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<td>Excitations are from this state.</td>
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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) (AG) (B3G) (B2U)
           (B3U) (B2G) (B1U) (AG) (B1U) (B2U) (AG)
           (B1U) (B1G) (B3U) (B3G) (AG) (B3G) (AG) (B2U)
           (B1U) (B2G) (B2U) (B3G) (B1G) (B1U) (B2G) (AU)
           (AG) (B3G) (B1U) (AG) (B2U) (B1U) (B3G) (AG) (B1U)
           (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   0.03845   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   0.87168
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):

Condensed to atoms (all electrons):

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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:

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Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

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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):

\(XXX= 0.0000\ YYY= 0.0000\ ZZZ= 0.0000\ XYY= 0.0000\)

\(XYX= 0.0000\ XZZ= 0.0000\ YYZ= 0.0000\)

\(XYZ= 0.0000\ YZX= 0.0000\ ZXY= 0.0000\)

Hexadecapole moment (field-independent basis, Debye-Ang**3):

\(XXXX= -21.6535\ YYYY= -27.0739\ ZZZZ= -68.5119\ XXXY= 0.0000\)

\(XXZX= 0.0000\ YYX= 0.0000\ YYYZ= 0.0000\ ZZZX= 0.0000\)

\(ZZZY= 0.0000\ XXYY= -8.8502\ XXZZ= -16.1757\ YYZZ= -13.1232\)

\(XYYX= 0.0000\ YZX= 0.0000\ ZXY= 0.0000\)

N-N= 3.324999423628D+01  E-N=-2.476162242765D+02  KE= 7.785168423628D+01
We find comfort among those who agree with us -- growth among those who don't.
-- Frank A. Clark

Job cpu time: 0 days 0 hours 8 minutes 54.9 seconds.
File lengths (MBytes): RWF=667 Int=0 D2E=0 Chk=16 Scr=48

Normal termination of Gaussian 03 at Sat May 10 12:39:06 2003.

### Output 637 ###

Entering Gaussian System, Link 0=/disk0/g03/g03/g03
Initial command:
/disk0/g03/g03/l1.exe /work/g03/inputs/Gau-53014.inp -scrdir=/work/g03/inputs/
Entering Link 1 = /disk0/g03/g03/l1.exe PID=53015.

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Cite this work as:
Gaussian 03, Revision B.01,
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,
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.
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Deg. of freedom  19
Full point group  D2H   NOp   8
Largest Abelian subgroup D2H   NOp   8
Largest concise Abelian subgroup D2   NOp   4

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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.

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.

\[ \text{NAtoms}=38 \quad \text{NActive}=38 \quad \text{NUuniq}=11 \quad \text{SFac}=5.66D+00 \quad \text{NAtFMM}=60 \quad \text{Big}=F \]

One-electron integrals computed using PRISM.

\[ \text{NBasis}=268 \quad \text{RedAO}=T \quad \text{NBF}=60 \quad 12 \quad 12 \quad 50 \quad 10 \quad 56 \quad 54 \quad 14 \]

\[ \text{NBsUse}=268 \quad \text{1.00D-06}=60 \quad 12 \quad 12 \quad 50 \quad 10 \quad 56 \quad 54 \quad 14 \]

\[ \text{Harris functional with IExCor}=205 \quad \text{AccDes}=1.00D-06 \quad \text{IRadAn}=1 \quad \text{IDoV}=1 \]

\[ \text{ScaDFX}=1.000000 \quad 1.000000 \quad 1.000000 \quad 1.000000 \]

Initial guess orbital symmetries:

**Occupied**

- \((B1U)\) \((AG)\) \((B2U)\) \((AG)\) \((B1U)\) \((AG)\) \((B3G)\) \((B1U)\) \((B2U)\)
- \((B2U)\) \((AG)\) \((B3G)\) \((B2U)\) \((B3G)\) \((B1U)\) \((B2U)\) \((B3G)\)
- \((B1U)\) \((AG)\) \((B3G)\) \((B2U)\) \((B1U)\) \((B2U)\) \((B3G)\) \((B1U)\)
- \((B2U)\) \((AG)\) \((B1U)\) \((B2U)\) \((B1U)\) \((B2U)\) \((B3G)\) \((B2U)\)
- \((B3G)\) \((B3G)\) \((B2U)\) \((B1U)\) \((B2U)\) \((B3G)\) \((B1U)\) \((B3G)\)

**Virtual**

- \((B2U)\) \((B1U)\) \((B1U)\) \((B2U)\) \((B1U)\) \((B2U)\) \((B1U)\) \((B2U)\)
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=  86643020

LASXX=  40755181 LTotXX=  40755181 LenRXX=  40755181

LTotAB=  0 MaxLAS=  179189010 LenRX=  0

NonZer=  81510362 LenScr=  123014144 LnRSAI=  356756400

LnScr1=  539029504 LExtra=  0 Total=  105955229

MaxDsk= -1 SrtSym=                T Tran=     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. Ebara, 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 = 40755181 NBLK = 25471 KOUNT = 1581

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, 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
### Linked Operators for SAC-CI: Symmetry = B2u Excited State

#### Main Reference Configuration and Coefficient

**1-st State**

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**2-nd State**

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**Selection**

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### Linked Operators for SAC-CI: Symmetry = B3u Excited State

#### Main Reference Configuration and Coefficient

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**2-nd State**

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**3-nd State**

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**Selection**

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### Step #CIMX# CI Matrix Elements

#### Singlet State

---

### Step #DIAGCI# Solution of SDI
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 WA VE 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

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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  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
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  -0.03948
79  84  -0.09911

**DOUBLE EXCITATION**
81  82  79  82  0.11164        80  83  79  82  0.09780
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  0.03661
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
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**DOUBLE EXCITATION**

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### 4-th ###

--- 9th state in this spin multiplicity ---

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**SINGLE EXCITATION**

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 Singlet      B2U  ************************************************************

### 1-st ###

--- 2nd state in this spin multiplicity ---

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**SINGLE EXCITATION**

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 Singlet      B2U  ************************************************************

### 3-rd ###

--- 3rd state in this spin multiplicity ---

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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
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
67  83  0.06115

*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
80  83  0.20963
76  84  0.09242
**Singlet B3U**

### 1-st ###           ---   7th state in this spin multiplicity ---

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Copying SAC-CI densities to excited state density rwf.
0 densities were copied.

******************************************************************************
Population analysis using the SCF density.
******************************************************************************

Orbital symmetries:

Occupied

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(B1U) (AG) (B2U) (AG) (B1U) (B3G) (B2U) (AG) (B1U)
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(B2U) (AG) (B3G) (B2U) (AG) (B1U) (B1U) (B2U)
(AG) (AG) (B3G) (B2U) (B1U) (B3G) (AG) (B1U) (B2U)
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(B2G) (B2G) (B3U) (B1G) (B3U) (AU)

Virtual

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(B2U) (AG) (B3G) (B1U) (B2U) (B3G) (AG) (AG) (B1U)

II
The electronic state is 1-AG.

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Alpha virt. eigenvalues --   10.69451  10.77105  10.83726  10.85387  10.85642
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| 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 | 0.000039  | -0.000012 | 0.000040  | 0.000041  | 0.000001  |
| 6  | C    | -0.000040 | -0.000020 | 0.000040 | -0.000011 | 0.000005 | -0.000012 |
| 7  | C    | -0.000040 | -0.000020 | 0.000040 | -0.000011 | 0.000005 | -0.000012 |
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| 9  | N    | -0.000040 | -0.000020 | 0.000040 | -0.000011 | 0.000005 | -0.000012 |
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<td>19</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>20</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>21</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>22</td>
<td>C</td>
<td>-0.088316</td>
</tr>
<tr>
<td>23</td>
<td>C</td>
<td>-0.088316</td>
</tr>
<tr>
<td>24</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>25</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>26</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>27</td>
<td>C</td>
<td>-0.088540</td>
</tr>
<tr>
<td>28</td>
<td>C</td>
<td>-0.088540</td>
</tr>
<tr>
<td>29</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>30</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>31</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>32</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>33</td>
<td>C</td>
<td>-0.088316</td>
</tr>
<tr>
<td>34</td>
<td>C</td>
<td>-0.088316</td>
</tr>
<tr>
<td>35</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>36</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>37</td>
<td>H</td>
<td>0.000000</td>
</tr>
<tr>
<td>38</td>
<td>H</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

Sum of Mulliken charges= 0.00000

Electronic spatial extent (au): \(<R^2> = 7683.8276\)

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

- \(X = 0.0000\)
- \(Y = 0.0000\)
- \(Z = 0.0000\)
- \(\text{Tot} = 0.0000\)

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):

- \(XXX = 0.0000\)
- \(YYY = 0.0000\)
- \(ZZZ = 0.0000\)
- \(XYZ = 0.0000\)
- \(XYY = 0.0000\)
- \(XZZ = 0.0000\)
- \(YYZ = 0.0000\)
- \(YZZ = 0.0000\)
- \(ZZX = 0.0000\)
- \(XXY = -154.7557\)
- \(XXZ = -117.2677\)
- \(XXX = -107.1650\)
- \(YYYX = 0.0000\)
- \(YYZX = 0.0000\)
- \(ZZXY = 0.0000\)
- \(XXYY = 0.0000\)
- \(XXZZ = 0.0000\)
- \(YYZZ = 0.0000\)
- \(ZZXX = 0.0000\)
- \(XXXZ = 0.0000\)
- \(XXXX = -182.0508\)
- \(YYYY = -4819.9941\)
- \(ZZZZ = -4653.8027\)
- \(XXXY = -1062.3973\)
- \(XXZZ = -1064.4300\)
- \(YYZZ = -1512.0636\)

N-N= 1.847455698009D+03 E-N=-5.986066886369D+03 KE= 9.819911244482D+02

Symmetry AG KE= 2.884197450548D+02
Symmetry B1G KE= 6.70031888467D+00
Symmetry B2G KE= 6.998072363256D+00
Symmetry B3G KE= 1.875664889780D+02
Symmetry AU KE= 4.335606164031D+00
Symmetry B1U KE= 2.378452044070D+02
Symmetry B2U KE= 2.382526639122D+02
Symmetry B3U KE= 1.187302468450D+01
Test job not archived.

$\text{1¥1¥GINC-MIRA18¥SP¥RSACC¥Gen¥C20H14N4¥MASAH¥31-Mar-2003¥0¥¥# SAC-}
\text{CI(SINGLET=(NSTATE=(0,0,0,0,4,4,1)), LEVELONE,WINDOW=(25,244))/GEN T}
\text{EST¥¥Gaussian Test Job 637: SAC-CI SD-R LevelOne calculation of optica}
\text{lly-allowed singlet excited states of Free-Base Porphin using Huzinaga}
\text{basis sets [4s2p/2s]. Inner-shells are excluded from the active space}
\text{and full-valence active MOs are used (FC; default): 57 occupied and 163}
\text{unoccupied MOs are included in the active space of SAC-CI. CPU memo}
\text{ry of 700MB is specified with %mem to allocate electron repulsion inte}
\text{grals in core memory (all ERIs are stored on cpu). If the core memory}
\text{is not enough for allocating all the repulsion integrals, according to}
\text{the available memory, the program will automatically divide the integ}
\text{ral file into appropriate number of files which are sequentially alloc}
\text{ated on the core memory. Experimental results and the results of Level}
\text{Two calculations are compared in Pa¥¥0,1¥N,0,2.122283,0.,0.YC,0,2.9039}
\text{91,1.131654,0.YC,0.2.43106,2.448915,0.YC,0,1.087013,2.860819,0.YN,0.0,}
\text{.2.032117,0.YC,0,-1.087013,2.860819,0.YC,0,-2.43106,2.448915,0.YC,0,-2}
\text{.903991,1.131654,0.YN,0,-2.122283,0.,0.YC,0,-2.903991,-1.131654,0.YC,0,}
\text{-2.43106,-2.448915,0.YC,0,-1.087013,-2.860819,0.YN,0.0,-2.032117,0.Y}
\text{C,0,1.087013,-2.860819,0.YC,0,2.43106,-2.448915,0.YC,0,2.903991,-1.131}
\text{654,0.YC,0.4.274858,-0.690194,0.YC,0.4.274858,0.690194,0.YH,0.5.131714}
\text{,1.353489,0.YH,0.5.131714,-1.353489,0.YH,0.3.188699,-3.229008,0.YC,0,0,}
\text{.682348,-4.268828,0.YC,0,0.682348,-4.268828,0.YH,0,1.357121,-5.11833}
\text{7,0.YH,0,1.357121,-5.118337,0.YH,0,-3.188699,-3.229008,0.YC,0,-4.274858}
\text{,8,-0.690194,0.YC,0,-4.274858,0.690194,0.YH,0,-5.131714,1.353489,0.YH,0}
\text{-5.131714,-1.353489,0.YH,0,-1.106269,0.0,YH,0,-3.188699,3.229008,0.YC,0}
\text{,-1.351714,-1.353489,0.YH,0,-1.106269,0.0,YH,0,-3.188699,3.229008,0.Y}
\text{C,0,-0.682348,4.268828,0.YC,0,-0.682348,4.268828,0.YH,0,1.357121,5.1183}
\text{837,0.YH,0,1.357121,5.118337,0.YH,0,3.188699,3.229008,0.YH,0,1.106269,0}
\text{,0.0¥¥Version=DEC-AXP-OSF/1-G03RevB.01¥State=1-AG¥HF=-982.9254061¥RMS}
\text{D=7.737e-09¥PG=D02H [C2(N1.N1),C2"(N1H1.H1N1),SG(C20H12)]¥¥@}

CONTRAIWISE...CONTINUED TWEEDLEDEE, IF IT WAS SO, IT MIGHT BE,
AND IF IT WERE SO, IT WOULD BE.....
BUT AS IT ISN'T, IT AIN'T....
THAT'S LOGIC.....
ALICE THROUGH THE LOOKING GLASS

Job cpu time: 0 days 2 hours 47 minutes 39.3 seconds.

File lengths (MBytes): RWF= 8139 Int= 0 D2E= 0 Chk= 46 Scr= 1363

### Output 638 ###

Entering Gaussian System, Link 0=/disk0/g03/g03/g03
Initial command:
/disk0/g03/g03/l1.exe /work/g03/inputs/Gau-53918.inp -scrdir=/work/g03/inputs/
Entering Link 1 = /disk0/g03/g03/l1.exe PID= 53919.
Warning -- This program may not be used in any manner that
competes with the business of Gaussian, Inc. or will provide
assistance to any competitor of Gaussian, Inc. The licensee
of this program is prohibited from giving any competitor of
Gaussian, Inc. access to this program. By using this program,
the user acknowledges that Gaussian, Inc. is engaged in the
business of creating and licensing software in the field of
computational chemistry and represents and warrants to the
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.

Cite this work as:
Gaussian 03, Revision B.01,
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 03: DEC-AXP-OSF/1-G03RevB.01 3-Mar-2003
31-Mar-2003

%mem=12mw

# SAC-CI(Singlet=(NState=(0,1)), TargetState=(SpinState=Singlet,Symmetry=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=90,40=1,41=2,42=2/1,4;
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.

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
C
F 1 FC
H 1 HC 2 HCF
Variables:
FC 1.308
HC 1.063
HCF 123.8

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

! Initial Parameters !
! (Angstroms and Degrees) !

! Name Definition Value Derivative Info. !
Input orientation:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
<td>0</td>
<td>0.000000 0.000000 0.000000</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>0</td>
<td>0.000000 0.000000 1.308000</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>0.883336 0.000000 -0.591342</td>
</tr>
</tbody>
</table>

Distance matrix (angstroms):

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>C</td>
<td>0.000000</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>F</td>
<td>1.308000 0.000000</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>H</td>
<td>1.063000 2.094704 0.000000</td>
<td></td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
<td>0</td>
<td>0.055209 0.698791 0.000000</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>0</td>
<td>0.055209 -0.609209 0.000000</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>-0.828128 1.290133 0.000000</td>
</tr>
</tbody>
</table>

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'')

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
Range of M.O.s used for correlation: 1 34
Use canonical orbitals as reference of MOD.
NBasis= 34 NAE= 8 NBE= 8 NFC= 0 NFV= 0
NROrb= 34 NOA= 8 NOB= 8 NVA= 26 NVB= 26

---------------------------------------------------------------------------------------------------------------
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 = 96814 NBLK = 60 KOUNT = 814

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 ==

<table>
<thead>
<tr>
<th></th>
<th>AG</th>
<th>AU</th>
</tr>
</thead>
<tbody>
<tr>
<td>SINGLET</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>TRIPLET</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>IONIZED</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>ANIONIZED</td>
<td>No</td>
<td>No</td>
</tr>
</tbody>
</table>

== 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

<table>
<thead>
<tr>
<th>LINKED OPERATORS FOR SAC: SYMMETRY = A'  GROUND STATE</th>
</tr>
</thead>
<tbody>
<tr>
<td>SELECTION</td>
</tr>
<tr>
<td>BEFORE</td>
</tr>
<tr>
<td>AFTER</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LINKED OPERATORS FOR SAC-CI: SYMMETRY = A&quot; EXCITED STATE</th>
</tr>
</thead>
<tbody>
<tr>
<td>#SECI# Main reference configuration and coefficient</td>
</tr>
<tr>
<td>## 1-st state ##  energy (au) = 0.060599</td>
</tr>
<tr>
<td>8 -&gt; 9  0.97258  8 -&gt; 13 -0.21751</td>
</tr>
<tr>
<td>SELECTION</td>
</tr>
<tr>
<td>BEFORE</td>
</tr>
<tr>
<td>AFTER</td>
</tr>
</tbody>
</table>

STEP #CIMX#  CI matrix elements

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=  -0.305242 (AU)
TOTAL ENERGY =  -138.076678 (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

STEP #SCIV# Iterative Diagonalization of SAC-CI-V

Threshold for density convergence (DConvDiag) .100D-04
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 =  -138.010848
Correlation energy in au =  -0.239412
Excitation energy in au =  0.065830    in eV =  1.791332

*SINGLE EXCITATION
  8   9   0.96020       8   13   -0.20874
  7   9   -0.04894       4   9   -0.03083

*DOUBLE EXCITATION
  8   23   8   9   0.06175       8   13   8   12   -0.05307
  8   14   8   13   -0.03744       6   9   5   9   0.03624
  8   23   4   9   0.03565       8   9   6   9   0.03178

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)= -0.2394122324 Total energy= -138.0108480242
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
1 Transform orbital 1 to 34
Compute gradients with respect to orbital rotations.
Differentiating once with respect to electric field.
with respect to dipole field.
Differentiating once with respect to nuclear coordinates.
Store integrals in memory, NReq= 997831.
Re-canonicalize molecular orbital basis.
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= 2.91D-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') (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') (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):

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>5.518680</td>
<td>0.219759</td>
<td>0.239722</td>
</tr>
<tr>
<td>F</td>
<td>0.219759</td>
<td>8.994027</td>
<td>-0.020415</td>
</tr>
<tr>
<td>H</td>
<td>0.239722</td>
<td>-0.020415</td>
<td>0.609163</td>
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</table>

Mulliken atomic charges:

<table>
<thead>
<tr>
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<th>3</th>
</tr>
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<tbody>
<tr>
<td>C</td>
<td>0.021839</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-0.193370</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.171531</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Sum of Mulliken charges= 0.0000

Atomic charges with hydrogens summed into heavy atoms:

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.193370</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-0.193370</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.000000</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Sum of Mulliken charges= 0.0000

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 YYY= -43.8399 ZZZ= -7.4060 XXY= -0.6004
XXXZ= 0.0000 YYYX= -3.2017 YYYZ= 0.0000 ZZZX= 0.0000
ZZZY= 0.0000 XXZY= -10.6749 XXZZ= -3.8509 YYZZ= -8.4109
XYYX= 0.0000 YYXZ= 0.0000 YZZX= -0.0163

N-N= 2.710729106638D+01  E-N=-3.817305559666D+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        -0.022660440  0.000000000  0.013031461
2        9         0.000068371  0.000000000  0.003044332
3        1         0.022592069  0.000000000 -0.016075792

Cartesian Forces:  Max  0.022660440  RMS  0.012742840

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces:  Max  0.027856408  RMS  0.016179129
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:

<table>
<thead>
<tr>
<th></th>
<th>R1</th>
<th>R2</th>
<th>A1</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>0.65019</td>
<td></td>
<td></td>
</tr>
<tr>
<td>R2</td>
<td>0.00000</td>
<td>0.38129</td>
<td></td>
</tr>
<tr>
<td>A1</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.16000</td>
</tr>
</tbody>
</table>

Eigenvalues --- 0.16000  0.38129  0.65019
RFO step:  Lambda=-2.04194017D-03.
Linear search not attempted -- first point.
Iteration 1 RMS(Cart)= 0.03491615  RMS(Int)= 0.00017116
Iteration 2 RMS(Cart)= 0.00018426  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  0.00293  0.00000  0.00449  0.00449  2.47626
R2        2.00878  0.02786  0.00000  0.07267  0.07267  2.08145
A1        2.16072  0.00085  0.00000  0.00525  0.00525  2.16597

Item  Value  Threshold  Converged?
Maximum Force  0.027856  0.000450  NO
RMS Force      0.016179  0.000300  NO
Maximum Displacement  0.038106  0.001800  NO
RMS Displacement  0.034987  0.001200  NO
Predicted change in Energy=-1.026410D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

|   | Center  Atomic  Atomic  Coordinates (Angstroms)
|---|Number  Number    Type    X       Y       Z|
|---|-------------|----------|---------|-------|-------|-------|
| 1 | 6          0        0  -0.010301  0.000000  0.008897|
| 2 | 9          0        0  -0.006172  0.000000  1.319268|
| 3 | 1          0        0   0.899810  0.000000 -0.611507|
Distance matrix (angstroms):

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>C</td>
<td>0.000000</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>F</td>
<td>1.310378</td>
<td>0.000000</td>
</tr>
<tr>
<td>3</td>
<td>H</td>
<td>1.101455</td>
<td>2.132767</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>0</td>
<td>0.057004</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>0</td>
<td>0.057004</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>-0.855057</td>
</tr>
</tbody>
</table>

Rotational constants (GHZ): 725.1778283 34.3478905 32.7945822
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 26.9227910502 Hartrees.
NAtoms= 3 NActive= 3 NUuniq= 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')
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') (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) = -137.771669277 A.U. after 10 cycles
          Conv =  0.9437D-08
          S**2   =  0.0000
Range of M.O.s used for correlation:  1  34
Transform orbitals by the MOD method.
  Overlap analysis:  1 - Trace/N =  0.000479
     Max |<i|j> - 1| =  0.002989
     Max <i|j>   =  0.002737
     Min eigenvalue =  0.996124
  Overlap analysis:  1 - Trace/N =-0.003776
     Max |<i|j> - 1| =  0.040254
     Max <i|j>   =  0.020708
     Min eigenvalue =  0.935718
NBasis=  34 NAE=  8 NBE=  8 NFC=  0 NFV=  0
NROrb=  34 NOA=  8 NOB=  8 NVA= 26 NVB=  26
  Non-canonical MOs are used.
  No. of INTEGRALS =  96814 NBLK =  60 KOUNT =  814
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 ###
---------------------------------------------------------------------------------------------------

II
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     =    -137.771669 (AU)
SAC-NV  ENERGY=      -0.306428 (AU)
TOTAL ENERGY  =    -138.078097 (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 =    -138.011827
Correlation energy in au =      -0.240158
Excitation energy  in au =       0.066270    in eV =       1.803303
**SINGLE EXCITATION**
  8    9     0.95947         8   13    -0.20831
  7    9    -0.05598         4    9    -0.03618
**DOUBLE EXCITATION**
  8   23    8    9     0.06178         8   13    8   12    -0.05303
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)= -0.2401575267 Total energy= -138.0118268032
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
  1 Transform orbital  1 to  34
Compute gradients with respect to orbital rotations.
    Differentiating once with respect to electric field.
        with respect to dipole field.
    Differentiating once with respect to nuclear coordinates.
Store integrals in memory, NReq=  997831.
Linear eq. for MOD by SimEqn.
Linear eq. for MOD by SimEqn.
Re-canonicalize molecular orbital basis.

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= 3.41D-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 *****

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>X Forces (Hartrees/Bohr)</th>
<th>Y Forces (Hartrees/Bohr)</th>
<th>Z Forces (Hartrees/Bohr)</th>
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<tbody>
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<td>-0.000738842</td>
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<td>Atomic Number</td>
<td>Atomic Number</td>
<td>Atomic Type</td>
<td>Coordinates (Angstroms)</td>
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<tr>
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<td>---------------</td>
<td>---------------</td>
<td>-------------</td>
<td>------------------------</td>
</tr>
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<td></td>
<td>X</td>
</tr>
<tr>
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<td>0</td>
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<td>0.000000</td>
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<tr>
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<td>9</td>
<td>0</td>
<td>-0.002839</td>
<td>0.000000</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>0.900649</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

Distance matrix (angstroms):

\[
\begin{bmatrix}
2 & 9 & 3 \\
2 & 9 & 3 \\
3 & 1 & 3 \\
\end{bmatrix}
\]
1  C  0.000000
2  F  1.310443  0.000000
3  H  1.102041  2.125964  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:

<table>
<thead>
<tr>
<th>Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
<td>0</td>
<td>0.057534 0.699256 0.000000</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>0</td>
<td>0.057534 -0.611187 0.000000</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>-0.863005 1.305147 0.000000</td>
</tr>
</tbody>
</table>

Rotational constants (GHZ):  710.3526120  34.4184611  32.8278643
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   26.9273163760 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')
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'') (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) = -137.773007292  A.U. after 9 cycles
Convg =  0.6678D-08  -V/T =  2.0006
S**2 =  0.0000
Range of M.O.s used for correlation:  1  34
Transform orbitals by the MOD method.
Overlap analysis:  1 - Trace/N =  0.000381
Max |<i|i> - 1| = 0.004176
Max <i|i> = 0.003043
Min eigenvalue = 0.995365
Overlap analysis: 1 - Trace/N = -0.003838
Max |<i|i> - 1| = 0.042651
Max <i|i> = 0.014987
Min eigenvalue = 0.937365

NBasis= 34 NAE= 8 NBE= 8 NFC= 0 NFV= 0
NROrb= 34 NOA= 8 NOB= 8 NVA= 26 NVB= 26
Non-canonical MOs are used.
No. of INTEGRALS = 96814 NBLK = 60 KOUNT = 814

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

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 = -137.773007 (AU)
SAC-NV ENERGY = -0.306403 (AU)
TOTAL ENERGY = -138.079411 (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 = -138.011838
Correlation energy in au = -0.238831
Excitation energy in au = 0.067572 in eV = 1.838736

*SINGLE EXCITATION
  8  9  0.95930  8  13  -0.20832
  7  9  -0.05891  4  9  -0.03491

*DOUBLE EXCITATION
  8  23  8  9  0.06170  8  13  8  12  -0.05286
  8  14  8  13  -0.03743  6  9  5  9  0.03606
  8  23  4  9  0.03522  8  9  6  9  0.03138

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)=   -0.2388309039 Total energy=      -138.0118381955
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
  1 Transform orbital   1 to   34
Compute gradients with respect to orbital rotations.
  Differentiating once with respect to electric field.
  with respect to dipole field.
  Differentiating once with respect to nuclear coordinates.
Store integrals in memory, NReq=      997831.
Linear eq. for MOD by SimEqn.
Linear eq. for MOD by SimEqn.
Re-canonicalize molecular orbital basis.
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= 5.36D-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 ******

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
<td>0.000193719</td>
<td>0.000000000</td>
<td>-0.000294825</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>0.000042070</td>
<td>0.000000000</td>
<td>0.000533938</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>-0.000235790</td>
<td>0.000000000</td>
<td>-0.000239113</td>
</tr>
</tbody>
</table>

Cartesian Forces:  Max  0.000533938  RMS  0.000241311

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces:  Max  0.000483329  RMS  0.000344511
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= 8.25D-01 RLast= 1.31D-02 DXMaxT set to 3.00D-01

The second derivative matrix:

<table>
<thead>
<tr>
<th></th>
<th>R1</th>
<th>R2</th>
<th>A1</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>0.65482</td>
<td></td>
<td></td>
</tr>
<tr>
<td>R2</td>
<td>-0.00816</td>
<td>0.38029</td>
<td></td>
</tr>
<tr>
<td>A1</td>
<td>0.03932</td>
<td>0.02758</td>
<td>0.19093</td>
</tr>
</tbody>
</table>

Eigenvalues --- 0.18359 0.38420 0.65825

RFO step: Lambda=-2.71690417D-07.
Quartic linear search produced a step of -0.14407.

Iteration 1 RMS(Cart)= 0.00124783 RMS(Int)= 0.00000073
Iteration 2 RMS(Cart)= 0.00000061 RMS(Int)= 0.00000000

Variable Old X -DE/DX Delta X Delta X Delta X New X
(R Linear) (Quad) (Total)
R1 2.47638 0.00048 -0.00002 0.00065 0.00063 2.47701
R2 2.08256 0.00000 -0.00016 0.00004 -0.00012 2.08243
A1 2.15291 0.00035 0.00188 -0.00012 0.00177 2.15467

Item Value Threshold Converged?
Maximum Force 0.000483 0.000450 NO
RMS Force 0.000345 0.000300 NO
Maximum Displacement 0.001267 0.001800 YES
RMS Displacement 0.001248 0.001200 NO

Predicted change in Energy=-4.537637D-07

Input orientation:

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

1 6 0 -0.013906 0.000000 0.006933
2 9 0 -0.003336 0.000000 1.317667
3 1 0 0.900579 0.000000 -0.607941

Distance matrix (angstroms):

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 C</td>
<td>0.000000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 F</td>
<td>1.310777</td>
<td>0.000000</td>
<td></td>
</tr>
<tr>
<td>3 H</td>
<td>1.101976</td>
<td>2.127211</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

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 | 0.057463 | 0.699344 | 0.000000 
2 | 9 | 0 | 0.057463 | -0.611432 | 0.000000 
3 | 1 | 0 | -0.861950 | 1.306824 | 0.000000 

Rotational constants (GHZ): 712.2763344 34.3920661 32.8079436
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 26.9206218760 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’)
 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) = -137.772809866 A.U. after 8 cycles
Conv = 0.7042D-08 -V/T = 2.0006
S**2 = 0.0000
Range of M.O.s used for correlation: 1 34
Transform orbitals by the MOD method.
Overlap analysis:

Overlap analysis:

<table>
<thead>
<tr>
<th>N Basis</th>
<th>NAE</th>
<th>NBE</th>
<th>NFC</th>
<th>NFV</th>
</tr>
</thead>
<tbody>
<tr>
<td>34</td>
<td>8</td>
<td>8</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>34</td>
<td>8</td>
<td>8</td>
<td>26</td>
<td>26</td>
</tr>
</tbody>
</table>

Non-canonical MOs are used.
No. of INTEGRALS = 96814 NBLK = 60 KOUNT = 814

**********************************************************************************
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

II
HF ENERGY = -137.772810 (AU)
SAC-NV ENERGY= -0.306422 (AU)
TOTAL ENERGY = -138.079232 (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 = -138.011839
Correlation energy in au = -0.239029
Excitation energy in au = 0.067393 in eV = 1.833858

*SINGLE EXCITATION*
8 9 0.95932 8 13 -0.20835
7 9 -0.05842 4 9 -0.03513

*DDOUBLE EXCITATION*
8 23 8 9 0.06171 8 13 8 12 -0.05287
8 14 8 13 -0.03742 6 9 5 9 0.03604
8 23 4 9 0.03521 8 9 6 9 0.03137

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) = -0.2390288220 Total energy = -138.0118386879
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
1 Transform orbital 1 to 34
Compute gradients with respect to orbital rotations.
Differentiating once with respect to electric field.
with respect to dipole field.
Differentiating once with respect to nuclear coordinates.
Store integrals in memory, NReq= 997831.
Linear eq. for MOD by SimEqn.
Linear eq. for MOD by SimEqn.
Re-canononicalize molecular orbital basis.
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.

Inv 2: IOpt= 1 Iter= 1 AM= 2.54D-16 Conv= 1.00D-12.
Inverted reduced A of dimension 12 with in-core refinement.
End of Minor Frequency-dependent properties file 721 does not exist.
***** Axes restored to original set *****

Center        Atomic   Force (Hartrees/Bohr)
Number        Number               X       Y       Z

<table>
<thead>
<tr>
<th>1</th>
<th>6</th>
<th>-0.000047590</th>
<th>0.000000000</th>
<th>-0.000006056</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>9</td>
<td>0.000212948</td>
<td>0.000000000</td>
<td>0.000116288</td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>-0.000165359</td>
<td>0.000000000</td>
<td>-0.000110232</td>
</tr>
</tbody>
</table>

Cartesian Forces: Max 0.000212948 RMS 0.000105760

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradBerny optimization.
Internal Forces: Max 0.000058779 RMS 0.000034551
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= 1.09D+00 RLast= 1.88D-03 DXMaxT set to 3.00D-01
The second derivative matrix:

<table>
<thead>
<tr>
<th>R1</th>
<th>R2</th>
<th>A1</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>0.59961</td>
<td></td>
</tr>
<tr>
<td>R2</td>
<td>-0.00262</td>
<td>0.38041</td>
</tr>
<tr>
<td>A1</td>
<td>0.02618</td>
<td>0.02901</td>
</tr>
</tbody>
</table>

Eigenvalues --- 0.19025 0.38487 0.60131
RFO step: Lambda= 0.00000000D+00.
Quartic linear search produced a step of 0.01951.
Iteration 1 RMS(Cart)= 0.000005054 RMS(Int)= 0.00000000
Iteration 2 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000000

<table>
<thead>
<tr>
<th>Variable</th>
<th>Old X</th>
<th>-DE/DX</th>
<th>Delta X</th>
<th>Delta X</th>
<th>Delta X</th>
<th>New X</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(Linear)</td>
<td>(Quad)</td>
<td>(Total)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R1</td>
<td>2.47701</td>
<td>0.00006</td>
<td>0.00001</td>
<td>0.00009</td>
<td>0.00010</td>
<td>2.47711</td>
</tr>
<tr>
<td>R2</td>
<td>2.08243</td>
<td>-0.00001</td>
<td>0.00000</td>
<td>-0.00001</td>
<td>-0.00001</td>
<td>2.08243</td>
</tr>
<tr>
<td>A1</td>
<td>2.15467</td>
<td>-0.00001</td>
<td>0.00003</td>
<td>-0.00010</td>
<td>-0.00007</td>
<td>2.15461</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Item</th>
<th>Value</th>
<th>Threshold</th>
<th>Converged?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum Force</td>
<td>0.000059</td>
<td>0.000450</td>
<td>YES</td>
</tr>
<tr>
<td>RMS Force</td>
<td>0.000035</td>
<td>0.000300</td>
<td>YES</td>
</tr>
<tr>
<td>Maximum Displacement</td>
<td>0.000061</td>
<td>0.001800</td>
<td>YES</td>
</tr>
<tr>
<td>RMS Displacement</td>
<td>0.000051</td>
<td>0.001200</td>
<td>YES</td>
</tr>
</tbody>
</table>

Predicted change in Energy=-3.289581D-09
Optimization completed.
-- Stationary point found.

! Optimized Parameters !
!(Angstroms and Degrees)!

! Name Definition Value Derivative Info. 
! R1 R(1,2) 1.3108 -DE/DX = 0.0001 
! R2 R(1,3) 1.1020 -DE/DX = 0.0 
! A1 A(2,1,3) 123.4538 -DE/DX = 0.0 

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms) X Y Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
<td>0</td>
<td>-0.013906 0.000000 0.006933</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>0</td>
<td>-0.003336 0.000000 1.317667</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>0.900579  0.000000 -0.607941</td>
</tr>
</tbody>
</table>

Distance matrix (angstroms):

<table>
<thead>
<tr>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 C 0.000000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 F 1.310777</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3 H 1.101976</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.127211</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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 Cl NOp 1

Standard orientation:

<table>
<thead>
<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Number</td>
<td>Number</td>
<td>Type</td>
<td>X</td>
</tr>
<tr>
<td>--------</td>
<td>--------</td>
<td>------</td>
<td>-------</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>0</td>
<td>0.057463</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>0</td>
<td>0.057463</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>-0.861950</td>
</tr>
</tbody>
</table>

Rotational constants (GHz): 712.2763344 34.3920661 32.8079436

Population analysis using the SCF density.

Orbital symmetries:

Occupied  (A') (A') (A') (A') (A') (A') (A')
Virtual    (A') (A') (A') (A') (A') (A') (A') (A') (A'') (A') (A') (A') (A') (A')

The electronic state is 1-A'.

Alpha occ. eigenvalues -- -26.35909 -11.36627 -1.67763 -0.92158 -0.76445
Alpha occ. eigenvalues -- -0.71460 -0.69896 -0.37535
Alpha virt. eigenvalues -- 0.07087 0.24883 0.35264 0.42798 0.49315
Alpha virt. eigenvalues -- 0.59775 0.67689 1.00946 1.11240 1.16348
Alpha virt. eigenvalues -- 1.21792 1.41601 1.73879 1.77981 1.78735
Alpha virt. eigenvalues -- 2.08567 2.27485 2.36115 2.40187 2.84368
Alpha virt. eigenvalues -- 2.93361 3.20566 4.03272 4.37125 27.38113
Alpha virt. eigenvalues -- 56.51011
Condensed to atoms (all electrons):
1  C   5.506545  0.217641  0.239962
2  F   0.217641  8.996980 -0.020734
3  H   0.239962 -0.020734  0.622738
Mulliken atomic charges:
1  C   0.035852
2  F  -0.193887
3  H   0.158034
Sum of Mulliken charges= 0.00000
Atomic charges with hydrogens summed into heavy atoms:
1  C   0.193887
2  F  -0.193887
3  H   0.000000
Sum of Mulliken charges= 0.00000
Electronic spatial extent (au): \(<R^2>= 56.7729\)
Charge= 0.0000 electrons
Dipole moment (field-independent basis, Debye):
X= -1.9207  Y= 0.4092  Z= 0.0000  Tot= 1.9638
### Quadrupole moment (field-independent basis, Debye-Ang):

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>XX</td>
<td>-12.2642</td>
</tr>
<tr>
<td>YY</td>
<td>-11.8047</td>
</tr>
<tr>
<td>ZZ</td>
<td>-10.0272</td>
</tr>
<tr>
<td>XY</td>
<td>-2.3852</td>
</tr>
<tr>
<td>XZ</td>
<td>0.0000</td>
</tr>
<tr>
<td>YZ</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

### Traceless Quadrupole moment (field-independent basis, Debye-Ang):

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>XX</td>
<td>-0.8988</td>
</tr>
<tr>
<td>YY</td>
<td>-0.4393</td>
</tr>
<tr>
<td>ZZ</td>
<td>1.3381</td>
</tr>
<tr>
<td>XY</td>
<td>-2.3852</td>
</tr>
<tr>
<td>XZ</td>
<td>0.0000</td>
</tr>
<tr>
<td>YZ</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

### Octapole moment (field-independent basis, Debye-Ang**2):

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>XXX</td>
<td>-1.9837</td>
</tr>
<tr>
<td>YYY</td>
<td>-6.9021</td>
</tr>
<tr>
<td>ZZZ</td>
<td>0.0000</td>
</tr>
<tr>
<td>XYY</td>
<td>-3.2603</td>
</tr>
<tr>
<td>XXXZ</td>
<td>-3.1727</td>
</tr>
<tr>
<td>XXZ</td>
<td>0.0000</td>
</tr>
<tr>
<td>XYZ</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

### Hexadecapole moment (field-independent basis, Debye-Ang**3):

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>XXXXX</td>
<td>-15.8985</td>
</tr>
<tr>
<td>YYYY</td>
<td>-44.3432</td>
</tr>
<tr>
<td>ZZZZ</td>
<td>0.0000</td>
</tr>
<tr>
<td>XXXXY</td>
<td>-3.2603</td>
</tr>
<tr>
<td>XXXXZ</td>
<td>-3.1727</td>
</tr>
<tr>
<td>YYYYX</td>
<td>-2.9275</td>
</tr>
<tr>
<td>YYYYZ</td>
<td>0.0000</td>
</tr>
<tr>
<td>XXYYZ</td>
<td>-3.9529</td>
</tr>
<tr>
<td>XXYXZ</td>
<td>0.0000</td>
</tr>
<tr>
<td>YYXZ</td>
<td>0.0000</td>
</tr>
<tr>
<td>ZZZX</td>
<td>-0.5332</td>
</tr>
<tr>
<td>ZZZY</td>
<td>-1.5724</td>
</tr>
<tr>
<td>XYZ</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

N-N= 2.692062187600D+01 E-N=-3.813185475723D+02  KE= 1.376875357949D+02

Symmetry A' KE= 1.317752389055D+02
Symmetry A" KE= 5.912296889344D+00

Final structure in terms of initial Z-matrix:

C
F,1,FC
H,1,HC,2,HCF

Variables:
FC=1.31077669
HC=1.10197636
HCF=123.45377038

Test job not archived.

MAN IS A SINGULAR CREATURE. HE HAS A SET OF GIFTS WHICH MAKE HIM UNIQUE AMONG THE ANIMALS: SO THAT, UNLIKE THEM, HE IS NOT A FIGURE IN THE LANDSCAPE -- HE IS A SHAPER OF THE LANDSCAPE.

-- JACOB BRONOWSKI

Job cpu time: 0 days 0 hours 10 minutes 7.2 seconds.

Initial command:
/disk0/g03/g03/l1.exe /work/g03/inputs/Gau-53918.inp -scrdir=/work/g03/inputs/
Entering Link 1 = /disk0/g03/g03/l1.exe PID= 53972.

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the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),
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Gaussian 03, Revision B.01,
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 03:  DEC-AXP-OSF/1-G03RevB.01 3-Mar-2003
31-Mar-2003
********************************************************************
%mem=12mw

# SAC-CI(SacOnly, TargetState=(SpinState=Singlet, Symmetry=1, Root=0)) / D95(d) Opt test
\[
\begin{align*}
1/18 &= 20, 38 = 1/1, 3; \\
2/9 &= 110, 17 = 5, 40 = 1/2; \\
3/5 &= 8, 7 = 1, 11 = 9, 16 = 1, 25 = 1, 30 = 1, 36 = 2/1, 2; \\
4/1 &= \\
5/5 &= 2, 38 = 5/2; \\
8/6 &= 5, 9 = 30000, 10 = 90, 40 = 1, 41 = 2, 42 = 2/1, 4; \\
9/15 &= 1/23; \\
11/28 &= -13, 29 = 200, 42 = 3, 46 = 2/11; \\
10/5 &= 5, 78 = 2/2; \\
6/7 &= 2, 8 = 2, 10 = 2/1; \\
7/12 &= 7/1, 2, 3, 16; \\
1/18 &= 20/3(1); \\
99/99 &= 2/9 = 110/2; \\
3/5 &= 8, 7 = 1, 11 = 9, 16 = 1, 25 = 1, 30 = 1, 36 = 2/1, 2; \\
4/5 &= 5, 16 = 3/1; \\
5/5 &= 2, 38 = 5/2; \\
8/6 &= 5, 9 = 30000, 10 = 90, 40 = 1, 41 = 2, 42 = 2/1, 4; \\
9/15 &= 1/23; \\
11/28 &= -13, 29 = 200, 42 = 3, 46 = 2/11; \\
10/5 &= 5, 78 = 2/2; \\
7/12 &= 7/1, 2, 3, 16; \\
1/18 &= 20/3(-9); \\
2/9 &= 110/2; \\
6/7 &= 2, 8 = 2, 9 = 2, 10 = 2/1; \\
99/99 &= \\
\end{align*}
\]

Gaussian Test Job 638 (Part 2): Geometry optimization of the SAC ground state of HCF. Initial geometry is the experimental one. MacroIter=1 (default).

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

\[
\begin{array}{ccc}
C & F & 1 & FC \\
H & 1 & HC & 2 & HCF \\
\end{array}
\]

Variables:

\[
\begin{align*}
FC &= 1.305 \\
HC &= 1.138 \\
HCF &= 104.1
\end{align*}
\]

Berny optimization.
Initialization pass.

--------

Initial Parameters

--------
! (Angstroms and Degrees) !

<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
<th>Value</th>
<th>Derivative Info.</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>R(1,2)</td>
<td>1.305</td>
<td>estimate D2E/DX2</td>
</tr>
<tr>
<td>R2</td>
<td>R(1,3)</td>
<td>1.138</td>
<td>estimate D2E/DX2</td>
</tr>
<tr>
<td>A1</td>
<td>A(2,1,3)</td>
<td>104.1</td>
<td>estimate D2E/DX2</td>
</tr>
</tbody>
</table>

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.

Input orientation:

<table>
<thead>
<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
<td>0</td>
<td>C</td>
<td>0.000000 0.000000 0.000000</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>0</td>
<td>F</td>
<td>1.305000 0.000000 1.305000</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>H</td>
<td>1.103714 0.000000 -0.277234</td>
</tr>
</tbody>
</table>

Distance matrix (angstroms):

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:

<table>
<thead>
<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
<td>0</td>
<td>C</td>
<td>0.068982 0.716735 0.000000</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>0</td>
<td>F</td>
<td>0.068982 -0.588265 0.000000</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>H</td>
<td>-1.034732 0.993969 0.000000</td>
</tr>
</tbody>
</table>

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')

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
Range of M.O.s used for correlation:  1  34
Use canonical orbitals as reference of MOD.
NBasis=  34 NAE=  8 NBE=  8 NFC=  0 NFV=  0
NROrb=  34 NOA=  8 NOB=  8 NVA=  26 NVB=  26

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,
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)

LINKED OPERATORS FOR SAC:

SYMMETRY = A’  GROUND STATE
SELECTION  SINGLE  DOUBLE  TOTAL
BEFORE  140  12216  12356
AFTER  140  4972  5113

STEP #CIMX#  CI matrix elements

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

HF ENERGY = -137.791947 (AU)
SAC-NV ENERGY= -0.307656 (AU)
TOTAL ENERGY = -138.099602 (AU)
SAC-NV coefficients (|C|>=0.03)
*SINGLE EXCITATION
  6    9      0.05294

*SINGLE EXCITATION
  8    9     8    9     -0.07927     8    9    7    9     0.05741
  8   13     8    9     0.05565     6   17     6    9    -0.05511
  8    9     4    9     -0.04798     6  17    5  18    -0.04540
  8   23     8    9     -0.04383     8   14     8   12    -0.03921
  6   17    6  17     -0.03855     7  9    4    9    0.03822
  6    9    6    9     -0.03766     6  17    4  16    -0.03369
  8   14    8    9     -0.03766     8   15    8   10    -0.03120
  7   14    8    9     -0.03075     8  11    8   11    -0.03069
  6    9    4  15     0.03066     8  11    7  11    -0.03056
  8   11     8   10     0.03022
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)= -0.3076558482 Total energy= -138.0996023721
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
  0 densities were copied.
Do SAC-NV density.
  1 Transform orbital 1 to 34
Compute gradients with respect to orbital rotations.
  Differentiating once with respect to electric field.
    with respect to dipole field.
  Differentiating once with respect to nuclear coordinates.
  Store integrals in memory, NReq= 997831.
  Re-canonicalize molecular orbital basis.
  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 = 4.38D-16 Conv = 1.00D-12.
Inverted reduced A of dimension 11 with in-core refinement.
End of Minor Frequency-dependent properties file 721 does not exist.

**********************************************************************

Population analysis using the SCF density.

**********************************************************************

Orbital symmetries:
Occupied (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')

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):

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>C</td>
<td>5.412807</td>
<td>0.228755</td>
</tr>
<tr>
<td>2</td>
<td>F</td>
<td>0.228755</td>
<td>9.013329</td>
</tr>
<tr>
<td>3</td>
<td>H</td>
<td>0.277592</td>
<td>-0.044807</td>
</tr>
</tbody>
</table>

Mulliken atomic charges:

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>C</td>
<td>0.080846</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>F</td>
<td>-0.197277</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>H</td>
<td>0.116431</td>
<td></td>
</tr>
</tbody>
</table>

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

<table>
<thead>
<tr>
<th></th>
<th>1</th>
</tr>
</thead>
</table>
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= -0.3227  YYZZ= -8.1525
  XXYZ= 0.0000  XXYZ= 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 *****

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Forces (Hartrees/Bohr) X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
<td>0.001355738</td>
<td>0.000000000</td>
<td>-0.017706500</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>0.003017516</td>
<td>0.000000000</td>
<td>0.011438935</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>-0.004373254</td>
<td>0.000000000</td>
<td>0.006267564</td>
</tr>
</tbody>
</table>

Cartesian Forces: Max 0.017706500 RMS 0.007555134

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.011729219 RMS 0.009337252
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:

<table>
<thead>
<tr>
<th></th>
<th>R1</th>
<th>R2</th>
<th>A1</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>0.65823</td>
<td></td>
<td></td>
</tr>
<tr>
<td>R2</td>
<td>0.00000</td>
<td>0.29807</td>
<td></td>
</tr>
<tr>
<td>A1</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.16000</td>
</tr>
</tbody>
</table>
Eigenvalues --- 0.16000 0.29807 0.65823
Linear search not attempted -- first point.
Iteration 1 RMS(Cart)= 0.04286608 RMS(Int)= 0.00088662
Iteration 2 RMS(Cart)= 0.00067952 RMS(Int)= 0.00000003
Iteration 3 RMS(Cart)= 0.00000004 RMS(Int)= 0.00000000
Variable Old X -DE/DX Delta X Delta X Delta X New X
(Linear) (Quad) (Total)
R1 2.46609 0.01173 0.00000 0.01780 0.01780 2.48389
R2 2.15051 -0.00610 0.00000 -0.02041 -0.02041 2.13010
A1 1.81689 -0.00931 0.00000 -0.05790 -0.05790 1.75899

Item Value Threshold Converged?
Maximum Force 0.011729 0.000450 NO
RMS Force 0.009337 0.000300 NO
Maximum Displacement 0.047888 0.001800 NO
RMS Displacement 0.043123 0.001200 NO
Predicted change in Energy=-4.380418D-04

GradGradGradGradGradGradGradGradGrad
Input orientation:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>0</td>
<td>-0.009026</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>0</td>
<td>0.019264</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>1.093476</td>
</tr>
</tbody>
</table>

Distance matrix (angstroms):

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>C</td>
<td>0.000000</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>F</td>
<td>1.314417</td>
<td>0.000000</td>
</tr>
<tr>
<td>3</td>
<td>H</td>
<td>1.127200</td>
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</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
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<tr>
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</tbody>
</table>

Rotational constants (GHZ): 458.9738440 36.5933755 33.8912696
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 27.0836614564 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”)
(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
ScFok: 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) = -137.792042807 A.U. after 10 cycles
Convg = 0.5330D-08 -V/T = 2.0005
S**2 = 0.0000
Range of M.O.s used for correlation: 1 34
Transform orbitals by the MOD method.
Overlap analysis:
Max |<i|i> - 1| = 0.003835
Max <i|i> = 0.005758
Min eigenvalue = 0.991471
Overlap analysis:
Max |<i|i> - 1| = 0.021361
Max <i|i> = 0.023358
Min eigenvalue = 0.960471
NBasis= 34 NAE= 8 NBE= 8 NFC= 0 NFV= 0
NROrb= 34 NOA= 8 NOB= 8 NVA= 26 NVB= 26
Non-canonical MOs are used.
No. of INTEGRALS = 96814 NBLK = 60 KOUNT = 814
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  No
TRIPLET  No  No
IONIZED  No  No
ANIONIZED No  No
== Input data for perturbation selection ==

SINGLET STATE
Number of States  Singlet  = ( 1, 0)
Threshold for perturbation selection of linked operator # LevelThree #
EThres2 (Lambda_G)= 0.100D-05 (au)  EThres2 (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  =  -137.792043 (AU)
SAC-NV ENERGY=      -0.307786 (AU)
TOTAL ENERGY  =    -138.099829 (AU)
SAC-NV coefficients (|C|>=0.03)
*SINGLE EXCITATION
  6   9   0.05374
*DOUBLE EXCITATION
  8   9   8   9   -0.07805
  6  17   6   9   -0.05520
  8   9   4   9   -0.04869
  8  23   8   9   -0.04378
  6  17  16  16   -0.03866
  6   9   6   9   -0.03771
  8   9   4  15   -0.04869
  8  17  17  17   -0.03866
  6  17   6  17   -0.03771
  8  14  14  14   -0.03357
  7   9  14  14   -0.03069
  8  14  14  14   -0.03357
  8   9   4  15   -0.04869
  8  14  14  14   -0.03357
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)=   -0.3077858508 Total energy=      -138.0998286573
Z-vector iteration converged.
Copying SAC-CI densities to excited state density r wf.
   0 densities were copied.
Do SAC-NV density.
  1 Transform orbital      1  to      34
Compute gradients with respect to orbital rotations.
   Differentiating once with respect to electric field.
      with respect to dipole field.
   Differentiating once with respect to nuclear coordinates.
Store integrals in memory, NReq=         997831.
Linear eq. for MOD by SimEqn.
Linear eq. for MOD by SimEqn.
Re-canonicalize molecular orbital basis.
   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= 3.27D-16 Conv= 1.00D-12.
Inverted reduced A of dimension 11 with in-core refinement.
End of Minor Frequency-dependent properties file 721 does not exist.
***** Axes restored to original set *****
-------------------------------------------------------------------
<table>
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<th>Center</th>
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<th>Forces (Hartrees/Bohr)</th>
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</thead>
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<tr>
<td>3</td>
<td>1</td>
<td>-0.000577671</td>
</tr>
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-------------------------------------------------------------------
Cartesian Forces: Max 0.006959232 RMS 0.003856644
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Broyden optimization.
Internal Forces: Max 0.009792587 RMS 0.007093207
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= 5.17D-01 RLast= 6.39D-02 DXMaxT set to 3.00D-01
The second derivative matrix:

R1 R2 A1
R1  0.51478
R2  0.06340  0.27944
A1  0.06111  0.01727  0.34270

Eigenvalues --- 0.26339 0.32333 0.55019
Quartic linear search produced a step of -0.32498.
Iteration 1 RMS(Cart)= 0.02117409 RMS(Int)= 0.00016648
Iteration 2 RMS(Cart)= 0.00012748 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
|---------|-------|--------|---------|---------|---------|-------
| R1      | 2.48389 | 0.00740 | -0.00578 | 0.01779 | 0.01201 | 2.49590 |
| R2      | 2.13010 | -0.00053 | 0.00663 | -0.01293 | -0.00630 | 2.12380 |
| A1      | 1.75899 | 0.00979 | 0.01882 | 0.00781 | 0.02662 | 1.78561 |

Item | Value | Threshold | Converged?
Maximum Force | 0.009793 | 0.000450 | NO
RMS Force | 0.007093 | 0.000300 | NO
Maximum Displacement | 0.021945 | 0.001800 | NO
RMS Displacement | 0.021129 | 0.001200 | NO

Predicted change in Energy=-1.769368D-04
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad


Input orientation:

<table>
<thead>
<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
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Distance matrix (angstroms):

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</thead>
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<td></td>
</tr>
<tr>
<td>2</td>
<td>1.320772 0.000000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1.123867 1.907971 0.000000</td>
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<td></td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
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<td>0</td>
<td>-1.029409</td>
</tr>
</tbody>
</table>

Rotational constants (GHZ): 468.6861629 36.0922776 33.5116355
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 26.9567802036 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') (A')
Virtual (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) = -137.792056073 A.U. after 9 cycles
Convg = 0.9333D-08 -V/T = 2.0006
S**2 = 0.0000
Range of M.O.s used for correlation: 1 34
Transform orbitals by the MOD method.
Overlap analysis:
Overlap analysis:
1 - Trace/N = -0.000048
Max |<i|j> - 1| = 0.003094
Max <i|j> = 0.003358
Min eigenvalue = 0.994807
Overlap analysis:
1 - Trace/N = -0.001495
Max |<i|j> - 1| = 0.020736
Max <i|j> = 0.013906
Min eigenvalue = 0.965497
NBasis= 34 NAE= 8 NBE= 8 NFC= 0 NFV= 0
NROrb= 34 NOA= 8 NOB= 8 NVA= 26 NVB= 26
Non-canonical MOs are used.
No. of INTEGRALS = 96814 NBLK = 60 KOUNT = 814
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)  EThres2 (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 = -137.792056 (AU)
SAC-NV ENERGY = -0.307930 (AU)
TOTAL ENERGY = -138.099986 (AU)

SAC-NV coefficients (|C|>=0.03)

*SINGLE EXCITATION
6 9 0.05417

*DOUBLE EXCITATION
8 9 8 9 -0.07901 8 9 7 9 0.05775
8 13 8 9 0.05576 6 17 6 9 -0.05507
8 9 4 9 -0.04832 6 17 5 18 -0.04569
8 23 8 9 -0.04379 8 14 8 12 -0.03875
6 17 6 17 -0.03875 7 9 4 9 0.03868
6 9 6 9 -0.03744 8 14 7 14 0.03396
6 17 4 16 -0.03381 8 15 8 10 -0.03191
7 14 6 9 -0.03080 6 9 4 15 0.03075

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)= -0.3079297696 Total energy= -138.0999858421
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
  0 densities were copied.
Do SAC-NV density.
    1    T r a n s f o r m  o r b i t a l      1  t o      3 4
Compute gradients with respect to orbital rotations.
    Differentiating once with respect to electric field.
    with respect to dipole field.
    Differentiating once with respect to nuclear coordinates.
    Store integrals in memory, NReq= 997831.
    Linear eq. for MOD by SimEqn.
    Linear eq. for MOD by SimEqn.
    Re-canonicalize molecular orbital basis.
    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= 3.38D-16 Conv= 1.00D-12.
Inverted reduced A of dimension 11 with in-core refinement.
End of Minor Frequency-dependent properties file  721 does not exist.
****** Axes restored to original set *****

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<th>Forces (Hartrees/Bohr)</th>
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<tr>
<td>3</td>
<td>1</td>
<td>0.001769620</td>
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</table>

Cartesian Forces: Max 0.001769620 RMS 0.000896722

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.001078436 RMS 0.000913320
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= 8.88D-01 RLast= 2.99D-02 DXMaxT set to 3.00D-01
The second derivative matrix:

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<tr>
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<th>R1</th>
<th>R2</th>
<th>A1</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>R2</td>
<td>0.02837</td>
<td>0.29955</td>
<td></td>
</tr>
<tr>
<td>A1</td>
<td>0.07974</td>
<td>-0.00222</td>
<td>0.35981</td>
</tr>
</tbody>
</table>

Eigenvalues --- 0.29261 0.33236 0.56159
RFO step: Lambda=-3.14636814D-06.
Quartic linear search produced a step of -0.09668.
Iteration 1 RMS(Cart)= 0.00186863 RMS(Int)= 0.00000118
Iteration 2 RMS(Cart)= 0.00000095 RMS(Int)= 0.00000000
Variable Old X -DE/DX Delta X Delta X Delta X New X
          (Linear) (Quad) (Total) (Total) (Total)
R1   2.49590 -0.00087 -0.00116 -0.00044 -0.00160 2.49429
R2   2.12380  0.00108  0.00061  0.00314  0.00375 2.12755
A1   1.78561 -0.00076 -0.00257  0.00082 -0.00175 1.78386

Item Value Threshold Converged?
Maximum Force 0.001078 0.000450 NO
RMS Force 0.000913 0.000300 NO
Maximum Displacement 0.002347 0.001800 NO
RMS Displacement 0.001869 0.001200 NO
Predicted change in Energy=-3.370215D-06
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Input orientation:
---------------------------------------------------------------------
<table>
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<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
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<tbody>
<tr>
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<td></td>
<td></td>
<td>X</td>
</tr>
</tbody>
</table>
---------------------------------------------------------------------
1       | 6             | 0             | -0.002361   | 0.000000   | -0.014467 |
2       | 9             | 0             | 0.010399    | 0.000000   | 1.305395  |
3       | 1             | 0             | 1.095677    | 0.000000   | -0.263162 |
---------------------------------------------------------------------
Distance matrix (angstroms):
1 2 3
1 0.000000
2 1.319924 0.000000
3 1.125849 1.907406 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

Standard orientation:

<table>
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<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
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<tr>
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</table>

Rotational constants (GHZ): 466.6025614 36.1448859 33.5462595

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 = 26.9664547833 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”) (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) = -137.792037422 A.U. after 8 cycles

Convg = 0.4520D-08 -V/T = 2.0006

S**2 = 0.0000

Range of M.O.s used for correlation: 1 34

Transform orbitals by the MOD method.

Overlap analysis:

1 - Trace/N = -0.000033

Max |<i|i> - 1| = 0.003196

Max <i|j> = 0.003485

Min eigenvalue = 0.994684

Overlap analysis:

1 - Trace/N = -0.001523

Max |<i|i> - 1| = 0.018706

Max <i|j> = 0.013401

Min eigenvalue = 0.966142

NBasis= 34 NAE= 8 NBE= 8 NFC= 0 NFV= 0
NROrb= 34 NOA= 8 NOB= 8 NVA= 26 NVB= 26
Non-canonical MOs are used.
No. of INTEGRALS = 96814 NBLK = 60 KOUNT = 814
*******************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R) Geometry optimization. IStep= 3
*******************************************************************************

== 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

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     =    -137.792037 (AU)
SAC-NV ENERGY=      -0.307952 (AU)
TOTAL ENERGY  =    -138.099989 (AU)
SAC-NV coefficients (|C|>=0.03)
*SINGLE EXCITATION
  6   9       0.05410
*DOUBLE EXCITATION
  8   9   8   9     -0.07891
  8  13   8   9       0.05570
  8   9   4   9     -0.04837
  8   23   8   9     -0.04380
  6   17   6   9     -0.03873
  6   9   6   9     -0.03747
  8   14   8   9     -0.03480
  6   17   6   9     -0.03873
  7   14   6   9     -0.03076
  6   9   4   15       0.03075
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)=   -0.3079517186 Total energy=      -138.0999891405
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
  0 densities were copied.
Do SAC-NV density.
  1 Transform orbital      1 to      34
Compute gradients with respect to orbital rotations.
  Differentiating once with respect to electric field.
  with respect to dipole field.
  Differentiating once with respect to nuclear coordinates.
Store integrals in memory, NReq=      997831.
Linear eq. for MOD by SimEqn.
Linear eq. for MOD by SimEqn.
  Re-canonicalize molecular orbital basis.
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= 6.90D-16 Conv= 1.00D-12.
Inverted reduced A of dimension 11 with in-core refinement.
End of Minor Frequency-dependent properties file 721 does not exist.
***** Axes restored to original set *****

<table>
<thead>
<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number</td>
<td>Number</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>0.000397286</td>
<td>0.0000000000</td>
<td>-0.000419412</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>-0.001053839</td>
<td>0.0000000000</td>
<td>-0.000387872</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0.000656553</td>
<td>0.0000000000</td>
<td>0.000807284</td>
</tr>
</tbody>
</table>

Cartesian Forces: Max 0.001053839 RMS 0.000545439

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.000010915 RMS 0.000009288
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= 9.79D-01 RLast= 4.43D-03 DXMaxT set to 3.00D-01
The second derivative matrix:

<table>
<thead>
<tr>
<th>R1</th>
<th>R2</th>
<th>A1</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>0.52586</td>
<td></td>
</tr>
<tr>
<td>R2</td>
<td>0.02662</td>
<td>0.30252</td>
</tr>
<tr>
<td>A1</td>
<td>0.07804</td>
<td>0.00076</td>
</tr>
</tbody>
</table>

Eigenvalues --- 0.29731 0.32907 0.55884
RFO step: Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.00455.
Iteration 1 RMS(Cart)= 0.00003185 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
<table>
<thead>
<tr>
<th></th>
<th>(Linear)</th>
<th>(Quad)</th>
<th>(Total)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>2.49429</td>
<td>0.00001</td>
<td>0.00001</td>
</tr>
<tr>
<td>R2</td>
<td>2.12755</td>
<td>-0.00001</td>
<td>-0.00002</td>
</tr>
<tr>
<td>A1</td>
<td>1.78386</td>
<td>-0.00001</td>
<td>-0.00001</td>
</tr>
</tbody>
</table>

Item                  Value Threshold Converged?
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum Force</td>
<td>0.000011</td>
<td>0.000450</td>
<td>YES</td>
</tr>
<tr>
<td>RMS Force</td>
<td>0.000009</td>
<td>0.000300</td>
<td>YES</td>
</tr>
<tr>
<td>Maximum Displacement</td>
<td>0.000034</td>
<td>0.001800</td>
<td>YES</td>
</tr>
<tr>
<td>RMS Displacement</td>
<td>0.000032</td>
<td>0.001200</td>
<td>YES</td>
</tr>
</tbody>
</table>
Predicted change in Energy=-4.236539D-10
Optimization completed.
-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
<th>Value</th>
<th>Derivative Info.</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>R(1,2)</td>
<td>1.3199</td>
<td>-DE/DX = 0.0</td>
</tr>
<tr>
<td>R2</td>
<td>R(1,3)</td>
<td>1.1258</td>
<td>-DE/DX = 0.0</td>
</tr>
<tr>
<td>A1</td>
<td>A(2,1,3)</td>
<td>102.2077</td>
<td>-DE/DX = 0.0</td>
</tr>
</tbody>
</table>

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Distance matrix (angstroms):

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>C</td>
<td>0.000000</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>F</td>
<td>1.319924</td>
<td>0.000000</td>
</tr>
<tr>
<td>3</td>
<td>H</td>
<td>1.125849</td>
<td>1.907406</td>
</tr>
</tbody>
</table>

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:

Rotational constants (GHZ): 466.6025614 36.1448859 33.5462595

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 --  -26.35025 -11.37604  -1.67215  -0.92475  -0.75858
Alpha occ. eigenvalues --   -0.70797  -0.66480  -0.41011
Alpha virt. eigenvalues --    0.06830   0.25475   0.32903   0.42310   0.49097
Alpha virt. eigenvalues --    1.20390  1.41991  1.74567  1.76188  1.77046
Alpha virt. eigenvalues --    2.05645  2.31370  2.36072  2.47261  2.83786
Alpha virt. eigenvalues --    2.83952  3.20170  4.01910  4.38573  27.37394
Alpha virt. eigenvalues --    56.52145

Condensed to atoms (all electrons):

1           2           3
1  C    5.401714   0.224205   0.281295
2  F    0.224205   9.038246  -0.046700
3  H    0.281295  -0.046700   0.642438

Mulliken atomic charges:

1
1  C    0.092785
2  F   -0.215752
3  H    0.122966

Sum of Mulliken charges=   0.00000

Atomic charges with hydrogens summed into heavy atoms:

1
1  C    0.215752
2  F   -0.215752
3  H    0.000000

Sum of Mulliken charges=   0.00000

Electronic spatial extent (au):  <R**2>=    55.6094

Charge=     0.0000 electrons

Dipole moment (field-independent basis, Debye):
X=   -1.5750  Y=    0.2290  Z=    0.0000  Tot=    1.5915

Quadrupole moment (field-independent basis, Debye-Ang):
XX=   -11.7153  YY=   -12.6763  ZZ=   -10.0496
XY=   -1.8539  XZ=    0.0000  YZ=    0.0000

Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX=   -0.2349  YY=   -1.1958  ZZ=    1.4308
XY=   -1.8539  XZ=    0.0000  YZ=    0.0000

Octapole moment (field-independent basis, Debye-Ang**2):
XXX=  -1.6982  YYY=   -8.6071  ZZZ=    0.0000  XYY=   -2.4682
XXY=  -1.8539  XXZ=    0.0000  XZZ=    0.3353  YZZ=    1.5613
YYZ=    0.0000  XYZ=    0.0000

Hexadecapole moment (field-independent basis, Debye-Ang**3):

II
XXX= -15.9355  YYYY= -45.4782  ZZZZ= -7.4579  XXXY= -0.3224
XXXZ= 0.0000  YYYY= -1.7829  ZZZX= 0.0000  ZZZY= 0.0000
ZZZY= 0.0000  XXYY= -10.7086  XXZZ= -4.0426  YYZZ= -8.1912  XXYZ= 0.0000  YYXZ= 0.0000
ZZXY= 0.1362

N-N= 2.696645478333D+01  KE= 1.377045822750D+02  Symmetry A'  KE= 1.318310990570D+02
Symmetry A"  KE= 5.873483217916D+00

Final structure in terms of initial Z-matrix:

<table>
<thead>
<tr>
<th>Element</th>
<th>Z-matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>1.31992379</td>
</tr>
<tr>
<td>F</td>
<td>1.12584893</td>
</tr>
<tr>
<td>H</td>
<td>102.20772317</td>
</tr>
</tbody>
</table>

Variables:

FC=1.31992379
HC=1.12584893
HCF=102.20772317

Test job not archived.

<table>
<thead>
<tr>
<th>Command Line</th>
<th>Gaussian Test Job 638 (Part 2): Geometry optimization of the SAC ground state of HCF. Initial geometry is the experimental one. MacroIter=1 (default).</th>
<th>Gaussian Test Job 638 (Part 2): Geometry optimization of the SAC ground state of HCF. Initial geometry is the experimental one. MacroIter=1 (default).</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU time</td>
<td>0 days 0 hours 8 minutes 45.1 seconds. File lengths (MBytes): RF= 457 Int= 0 D2E= 0 Chk= 10 Scr= 19 Normal termination of Gaussian 03 at Mon Mar 31 20:30:22 2003.</td>
<td>Normal termination of Gaussian 03 at Mon Mar 31 20:30:22 2003.</td>
</tr>
</tbody>
</table>

### Output 647 ###

Entering Gaussian System, Link 0=/disk0/g03/g03/g03
Initial command:
/disk0/g03/g03/l1.exe /work/g03/inputs/Gau-54596.inp -scrdir=/work/g03/inputs/
Entering Link 1 = /disk0/g03/g03/l1.exe PID= 54597.


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Cite this work as:
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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,
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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. Daubr, 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 03:  DEC-AXP-OSF/1-G03RevB.01 3-Mar-2003
31-Mar-2003
*************************************************

%mem=12mw

# SAC-CI(Singlet=(NState=(0,1,0,0)), TargetState=(SpinState=Singlet,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;
9/15=1/23;
11/28=-14,29=200,42=3,46=1/11;
10/5=5,78=1/2;
6/7=2,8=2,9=2,10=2/1;
7/12=7/1,2,3,16;
1/18=20/3(1);
\[
\begin{align*}
99/99; \\
2/9=110/2; \\
3/5=8,7=101,11=9,16=1,25=1,30=1,36=2/1,2,3; \\
4/5=5,16=3/1; \\
5/5=2,38=5/2; \\
8/6=5,9=3000,10=1,40=1,42=1/1,2,3; \\
9/15=1/23; \\
11/28=14,29=200,42=3,46=1/11; \\
10/5=5,78=1/2; \\
7/12=7/1,2,3,16; \\
1/18=20/3(-9); \\
2/9=110/2; \\
6/7=2,8=2,9=2,10=2/1; \\
99/99;
\end{align*}
\]

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 a 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.

Symbolic Z-matrix:

\[
\begin{align*}
\text{Charge} &= 0 \quad \text{Multiplicity} = 1 \\
B \\
H \\
\text{Variables:} \\
\quad BH \\
\quad 1.1963
\end{align*}
\]

Berny optimization. Initialization pass.

\[
\begin{align*}
\text{Trust Radius} &= 3.00D-01 \quad \text{FncErr} = 1.00D-07 \quad \text{GrdErr} = 1.00D-07 \\
\text{Number of steps in this run} &= 20 \quad \text{maximum allowed number of steps} = 100.
\end{align*}
\]

Input orientation:
<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>X</td>
<td>Y</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>0</td>
<td>0.000000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>X</td>
<td>Y</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>0</td>
<td>0.000000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

Rotational constants (GHZ): 0.0000000 382.4658857 382.4658857

Standard basis: D95(d,p) (6D, 7F)

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) (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) = -25.123368036 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=

AccDes= 0.00D+00

HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn=

ScaDFX= 1.000000 1.000000 1.000000

Range of M.O.s used for correlation: 2 20

N Basis = 21 NAE= 3 NBE= 3 NFC= 1 N FV= 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:

<table>
<thead>
<tr>
<th>SYMMETRY = A1</th>
<th>GROUND STATE</th>
</tr>
</thead>
<tbody>
<tr>
<td>SELECTION</td>
<td>SINGLE</td>
</tr>
<tr>
<td>BEFORE</td>
<td>16</td>
</tr>
<tr>
<td>AFTER</td>
<td>16</td>
</tr>
</tbody>
</table>

STEP #CIMX#  CI matrix elements

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
*******************************************************************************
S I N G L E T  S T A T E
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
S i n g l e t              0 1 0 0                  0 1 0 0                 3
Single
B-operator: SDCI for reference-CI with small active space
Generate all the higher-order excitation operators
Skip higher-order unlinked terms
*******************************************************************************
S I N G L E T  S T A T E
*******************************************************************************
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
3: 3 8 3 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

II
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

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 = -24.979507
Correlation energy in au = 0.143830
Excitation energy in au = 0.225392 in eV = 6.133238

*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) = 0.1438297461 Total energy = -24.9795070574
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
  1 Transform orbital  1 to  19
Compute gradients with respect to orbital rotations.
Evalate gradients in canonical representation.
CutOGr = 0.100D-08
  Differentiating once with respect to electric field.
  with respect to dipole field.
  Differentiating once with respect to nuclear coordinates.
  Store integrals in memory, NReq= 847198.
  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= 2.81D-16 Conv= 1.00D-12.
Inverted reduced A of dimension  8 with in-core refinement.
End of Minor 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) (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
  B  4.671320  0.299095
  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=  0.00000 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  YYYY=  0.0000  YYZZ=  0.0000  ZZZX=  0.0000
  YYYY=  0.0000  XXXY=  -2.8761  XXZZ=  -5.9830  YYZZ=  -5.9830
  XYYX=  0.0000  ZZZY=  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  0.000000000  0.001648658
2           1           0.000000000  0.000000000  0.000000000  0.001648658

Cartesian Forces:  Max  0.001648658 RMS  0.000951853

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Berny optimization.

Internal Forces:  Max  0.001648658 RMS  0.001648658
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:

\[
\begin{pmatrix}
R1 & 0.24937 \\
R1 & \\
Eigenvalues --- & 0.24937 \\
\end{pmatrix}
\]
RFO step: Lambda=-1.08991296D-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=-5.449803D-06

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Input orientation:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>0</td>
<td>0.000000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
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<tr>
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<td></td>
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<td>X</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>0</td>
<td>0.000000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

Rotational constants (GHZ): 0.0000000 380.2387674 380.2387674
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 2.2052756244 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) (SG) (SG) (SI) (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) = -25.1234383985 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 Occupied 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

*******************************************************************************
Singles-Doubles (SD) SAC/SAC-CI (SAC-CI SD-R) Geometry optimization. IStep= 1
*******************************************************************************

== States to be calculated ==
  A1  A2  B1  B2
SINGLET

SINGLET STATE

Threshold for perturbation selection of linked operator # LevelThree #
EThreS2 (Lambda_G)= 0.100D-05 (au)  EThreS2 (Lambda_E)= 0.100D-06 (au)

During geometry optimization, the same linked and unlinked operators are used.

***** SINGLET STATE *****

ENERGY AND WAVE FUNCTION OF SAC METHOD

HF ENERGY = -25.123438 (AU)
SAC-NV ENERGY= -0.081587 (AU)
TOTAL ENERGY = -25.205026 (AU)
Number of States Singlet \( = (0 1 0 0) \)

Perturbation selection with reference state

Threshold of perturbation selection of linked operator \# LevelThree \# 

\[ \text{ETHreR2(E)} (\text{Lambda}_E) = 0.100D-06(\text{au}) \]

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 \( (\text{CThreULR1}, \text{CThreULR2}) 0.500D-01 0.500D-01 \)

Threshold for S2 operators \( (\text{CThreULS2}) 0.000D+00 \)

STEP #SCIV# Iterative diagonalization OF SAC-CI-V

Threshold for density convergence \( (\text{DConvDiag}) .100D-04 \)

Maximum number of iteration \( (\text{MaxItDiag}) 64 \)

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 = 6.136533

*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
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)= 0.1439260547 Total energy= -24.9795123438
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
   1 Transform orbital 1 to 19
Compute gradients with respect to orbital rotations.
Evalate gradients in canonical representation.
CutOGr = 0.100D-08
   Differentiating once with respect to electric field.
      with respect to dipole field.
   Differentiating once with respect to nuclear coordinates.
Store integrals in memory, NReq= 847198.
    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= 3.15D-16 Conv= 1.00D-12.
Inverted reduced A of dimension 8 with in-core refinement.
End of Minor Frequency-dependent properties file 721 does not exist.
***** Axes restored to original set *****
Number      Number               X               Y               Z
-------------------------------------------------------------------
 1          5           0.000000000    0.000000000    0.000042303
 2          1           0.000000000    0.000000000   -0.000042303
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000042303 RMS     0.000024424
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces:  Max     0.000042303 RMS     0.000042303
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  0.25578

Eigenvalues ---  0.25578
RFO step:  Lambda= 0.00000000D+00.
Quartic linear search produced a step of -0.02533.
Iteration  1 RMS(Cart)=  0.00011839 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

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=-3.497620D-09
Optimization completed.
-- Stationary point found.

--- Optimized Parameters ---
--- (Angstroms and Degrees) ---

<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
<th>Value</th>
<th>Derivative Info.</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>R(1,2)</td>
<td>1.1998</td>
<td>-DE/DX = 0.0</td>
</tr>
</tbody>
</table>

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Input orientation:

 Center      Atomic      Atomic      Coordinates (Angstroms)
Number      Number      Type      X      Y      Z
-------------------------------------------------------------------
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:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>0</td>
<td>0.000000 0.000000 0.199966</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0</td>
<td>0.000000 0.000000 -0.999832</td>
</tr>
</tbody>
</table>

Rotational constants (GHZ):  0.0000000 380.2387674 380.2387674

Population analysis using the SCF density.

Orbital symmetries:

<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>The electronic state is 1-SG.</td>
<td></td>
</tr>
<tr>
<td>Alpha occ. eigenvalues --</td>
<td>-7.68845 -0.65888 -0.34292</td>
</tr>
<tr>
<td>Alpha virt. eigenvalues --</td>
<td>0.04879 0.04879 0.22494 0.35243 0.35243</td>
</tr>
<tr>
<td>Alpha virt. eigenvalues --</td>
<td>0.41147 0.47358 1.24503 1.59049 1.59049</td>
</tr>
<tr>
<td>Alpha virt. eigenvalues --</td>
<td>1.74805 1.74805 2.06287 2.45670 2.45670</td>
</tr>
<tr>
<td>Alpha virt. eigenvalues --</td>
<td>3.29485 4.76950 20.46680</td>
</tr>
</tbody>
</table>

Condensed to atoms (all electrons):

<table>
<thead>
<tr>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>4.670256 0.298848</td>
</tr>
<tr>
<td>H</td>
<td>0.298848 0.732049</td>
</tr>
</tbody>
</table>

Mulliken atomic charges:

<table>
<thead>
<tr>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>0.030896</td>
</tr>
<tr>
<td>H</td>
<td>-0.030896</td>
</tr>
</tbody>
</table>

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

<table>
<thead>
<tr>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>0.000000</td>
</tr>
<tr>
<td>H</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

Sum of Mulliken charges= 0.00000
Electronic spatial extent (au): \( <R^{**2}> = 21.8596 \)
Charge = 0.0000 electrons
Dipole moment (field-independent basis, Debye):
\[
X = 0.0000 \quad Y = 0.0000 \quad Z = -2.0772 \quad \text{Tot} = 2.0772
\]
Quadrupole moment (field-independent basis, Debye-Ang):
\[
XX = -6.5087 \quad YY = -6.5087 \quad ZZ = -10.6226
XY = 0.0000 \quad XZ = 0.0000 \quad YZ = 0.0000
\]
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
\[
XX = 1.3713 \quad YY = 1.3713 \quad ZZ = 2.7426
XY = 0.0000 \quad XZ = 0.0000 \quad YZ = 0.0000
\]
Octapole moment (field-independent basis, Debye-Ang**2):
\[
XXX = 0.0000 \quad YYY = 0.0000 \quad ZZZ = -6.5468 \quad XYY = 0.0000
XXX = 0.0000 \quad XXZ = -1.6039 \quad XZZ = 0.0000 \quad YZZ = 0.0000
YYY = 0.0000 \quad ZYY = 0.0000 \quad ZYZ = 0.0000 \quad ZZXY = 0.0000
XYZ = 0.0000 \quad YYZ = 0.0000 \quad YZX = 0.0000 \quad ZZYZ = 0.0000
XYZ = 0.0000 \quad XYZ = 0.0000 \quad XZZ = 0.0000 \quad YYY = 0.0000
ZZZ = -1.6039 \quad ZZY = 0.0000 \quad XXZ = -1.6039 \quad YYX = 0.0000
XXX = 0.0000 \quad YYZ = 0.0000 \quad ZYY = 0.0000 \quad XZZ = 0.0000
\]
Hexadecapole moment (field-independent basis, Debye-Ang**3):
\[
XXXX = -8.6322 \quad YYYY = -8.6322 \quad ZZZZ = -27.3257 \quad XXXY = 0.0000
XXXX = 0.0000 \quad XXXZ = -1.6039 \quad XXXZ = 0.0000 \quad XYYZ = 0.0000
YYYY = 0.0000 \quad YYYY = -2.8774 \quad XXZZ = 5.9963 \quad YYYZ = 5.9963
ZZZZ = 0.0000 \quad ZZZZ = 9.963 \quad YXYZ = 9.963 \quad XXZZ = 9.963
XXXZ = 0.0000 \quad XXXZ = 9.963 \quad XXXZ = 9.963 \quad XYYZ = 9.963
\]
N-N = 2.205275624387D+00 E-N = -6.24103534306D+01 KE = 2.513345967661D+01
Symmetry A1 KE = 2.513345967661D+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:

Test job not archived.

ON INDUCTION, OR "WHY DO YOU BELIEVE THE SUN WILL RISE TOMORROW?:"

... THE FARMER WHO HAS FED THE CHICKEN EVERY DAY THROUGHOUT ITS
LIFE AT LAST WRINGS ITS NECK INSTEAD, SHOWING THAT MORE REFINED VIEWS AS TO THE UNIFORMITY OF NATURE WOULD HAVE BEEN USEFUL TO THE CHICKEN.

-- BERTRAND RUSSELL

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
Initial command:
/disk0/g03/g03/l1.exe /work/g03/inputs/Gau-54596.inp -scrdir=/work/g03/inputs/
Entering Link 1 = /disk0/g03/g03/l1.exe PID= 54598.

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Gaussian, Inc.
Carnegie Office Park, Building 6, Pittsburgh, PA 15106 USA

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Cite this work as:
Gaussian 03, Revision B.01,
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 03: DEC-AXP-OSF/1-G03RevB.01 3-Mar-2003
31-Mar-2003
*************************************************
Warning: CPHF=MOD not CPHF=Canonical is strongly recommended with GSUM.

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.
Initial Parameters (Angstroms and Degrees)!

<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
<th>Value</th>
<th>Derivative Info.</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>R(1,2)</td>
<td>1.1963</td>
<td>estimate D2E/DX2</td>
</tr>
</tbody>
</table>

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.

Input orientation:

```
<table>
<thead>
<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td></td>
<td></td>
<td>X</td>
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<td>5</td>
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<td>0</td>
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</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0.000000</td>
</tr>
</tbody>
</table>
```

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:

```
<table>
<thead>
<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
</tr>
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<tbody>
<tr>
<td></td>
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<td>0.000000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0.000000</td>
</tr>
</tbody>
</table>
```

Rotational constants (GHZ): 0.000000 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.
N Basis = 21 RedAO = T NBF = 12 1 4 4
N Basis Use = 21 1.00D-06 NBFU = 12 1 4 4
Harris functional with IXCor = 205 diagonalized for initial guess.
Exp Min = 7.01D-02 Exp Max = 2.79D+03 Exp MxC = 4.19D+02 I Acc = 2 IRadAn =
Acc Des = 0.00D+00
HarFok: IX Cor = 205 Acc Des = 0.00D+00 IRadAn =
ScaDFX = 1.000000 1.000000 1.000000 1.000000
Initial guess orbital symmetries:
Occupied (SG) (SG) (SG)
Virtual (PI) (PI) (SG) (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, N Req = 871060.
SCF Done: E(RHF) = -25.1233368036 A.U. after 8 cycles
Conv g = 0.5126D-08 -V/T = 1.9995
S**2 = 0.0000
Perform MO ordering.
Exp Min = 7.01D-02 Exp Max = 2.79D+03 Exp MxC = 4.19D+02 I Acc = 3 IRadAn =
Acc Des = 0.00D+00
HarFok: IX Cor = 205 Acc Des = 0.00D+00 IRadAn =
ScaDFX = 1.000000 1.000000 1.000000 1.000000
Range of M.O.s used for correlation: 2 20
N Basis = 21 NAE = 3 NBE = 3 NFC = 1 NFV = 1
N ROrb = 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

SINGLET STATE

Number of States Singlet = ( 0 1 0 0 )
Perturbation selection with reference state
  Threshold of perturbation selection of linked operator # LevelThree #
  ETthreR2(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

<table>
<thead>
<tr>
<th>SELECTION</th>
<th>SINGLE</th>
<th>DOUBLE</th>
<th>TOTAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>BEFORE</td>
<td>2</td>
<td>96</td>
<td>98</td>
</tr>
</tbody>
</table>
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

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 = -24.955770
Correlation energy in au = 0.167567
Excitation energy in au = 0.249130 in eV = 6.779169

*SINGLE EXCITATION
3 15 -0.04676

*DOUBLE EXCITATION
3 5 3 4 0.89764 3 7 3 5 0.28790
3 8 3 4 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

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) = 0.1675672834 Total energy = -24.9557695202

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
1 Transform orbital 1 to 19

Compute gradients with respect to orbital rotations.
Evaluate gradients in canonical representation.
CutOGr = 0.100D-08
Differentiating once with respect to electric field.
with respect to dipole field.
Differentiating once with respect to nuclear coordinates.
Store integrals in memory, NReq= 847198.
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= 2.97D-16 Conv= 1.00D-12.
Inverted reduced A of dimension 8 with in-core refinement.
End of Minor 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) (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):

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>4.671320</td>
<td>0.299095</td>
</tr>
<tr>
<td>H</td>
<td>0.299095</td>
<td>0.730491</td>
</tr>
</tbody>
</table>

Mulliken atomic charges:

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>0.029585</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.029585</td>
<td></td>
</tr>
</tbody>
</table>

Sum of Mulliken charges= 0.00000

Atomic charges with hydrogens summed into heavy atoms:

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>0.00000</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.00000</td>
<td></td>
</tr>
</tbody>
</table>

Sum of Mulliken charges= 0.00000

Electronic spatial extent (au): \(<R^2>= 21.8244\)

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>X</td>
<td>0.0000</td>
<td>Y</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

Quadrupole moment (field-independent basis, Debye-Ang):

<p>| | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>XX</td>
<td>-6.5054</td>
<td>YY</td>
<td>-6.5054</td>
<td>ZZ</td>
<td>-10.6155</td>
<td></td>
</tr>
<tr>
<td>XY</td>
<td>0.0000</td>
<td>XZ</td>
<td>0.0000</td>
<td>YZ</td>
<td>0.0000</td>
<td></td>
</tr>
</tbody>
</table>

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
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<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>XX</td>
<td>1.3700</td>
<td>YY</td>
<td>1.3700</td>
<td>ZZ</td>
<td>-2.7401</td>
</tr>
<tr>
<td>XY</td>
<td>0.0000</td>
<td>XZ</td>
<td>0.0000</td>
<td>YZ</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

Octapole moment (field-independent basis, Debye-Ang**2):

<p>| | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>XXX</td>
<td>0.0000</td>
<td>YYYY</td>
<td>0.0000</td>
<td>ZZZ</td>
<td>-6.5665</td>
<td>XYY= 0.0000</td>
<td></td>
</tr>
<tr>
<td>XXY</td>
<td>0.0000</td>
<td>XXZ= -1.6113</td>
<td>XZZ= 0.0000</td>
<td>YZZ= 0.0000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>YYY</td>
<td>-1.6113</td>
<td>XYZ= 0.0000</td>
<td>XYY= 0.0000</td>
<td>XXZ= 0.0000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ZZZ</td>
<td>0.0000</td>
<td>ZZXY= 0.0000</td>
<td>YYYY= 0.0000</td>
<td>XXZ= 0.0000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>XYZ</td>
<td>0.0000</td>
<td>XXXY= 0.0000</td>
<td>YYYY= 0.0000</td>
<td>XXZ= 0.0000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>XYZ</td>
<td>0.0000</td>
<td>XXXZ= 0.0000</td>
<td>YYYY= 0.0000</td>
<td>XXZ= 0.0000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>YZZ</td>
<td>-5.9830</td>
<td>YZZ= -5.9830</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Hexadecapole moment (field-independent basis, Debye-Ang**3):

|   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| XXXX | -8.6284 | YYYY= -8.6284 | ZZZZ= -27.2484 | XXY= 0.0000 |
| XXXZ | 0.0000 | YYYY= 0.0000 | YYYY= 0.0000 | XXZ= 0.0000 |
| ZZZY | 0.0000 | YYYY= 0.0000 | YYYY= 0.0000 | XXZ= 0.0000 |
| ZZZX | 0.0000 | YYYY= 0.0000 | YYYY= 0.0000 | XXZ= 0.0000 |
| ZZYY | 0.0000 | YYYY= 0.0000 | YYYY= 0.0000 | XXZ= 0.0000 |
| XXXY | 0.0000 | YYYX= 0.0000 | YYYY= 0.0000 | XXZ= 0.0000 |
| XXXZ | 0.0000 | YYYX= 0.0000 | YYYY= 0.0000 | XXZ= 0.0000 |
| YYYY | 0.0000 | YYYX= 0.0000 | YYYY= 0.0000 | XXZ= 0.0000 |
| ZZZX | 0.0000 | YYYX= 0.0000 | YYYY= 0.0000 | XXZ= 0.0000 |
| ZZYY | 0.0000 | YYYX= 0.0000 | YYYY= 0.0000 | XXZ= 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 ****

---

<table>
<thead>
<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>0.000000000</td>
<td>0.000000000</td>
<td>-0.002894765</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.000000000</td>
<td>0.000000000</td>
<td>-0.002894765</td>
</tr>
</tbody>
</table>

Cartesian Forces: Max 0.002894765 RMS 0.001671293
Berny optimization.

Internal Forces: Max 0.002894765 RMS 0.002894765

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

Eigenvalues --- 0.24937

RFO step: Lambda=-3.35983544D-05.

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.00820710 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=-1.680144D-05

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): 0.000000 386.4235872 386.4235872
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 2.2231383694 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) (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) = -25.1231312157 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.

****************************
S I N G L E T  S T A T E
****************************

STEP #CIMX# CI matrix elements

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 #
  ETThreR2(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 STATE
一号 1-st 一号 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 = 6.771984

*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 4 2 8 -0.04180 3 5 2 7 -0.04180
3 13 2 4 0.03540 3 12 2 5 0.03540

================================================================
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)= 0.1673461530 Total energy= -24.9557850627
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
  1 Transform orbital 1 to 19
Compute gradients with respect to orbital rotations.
Evaluate gradients in canonical representation.
CutOGr = 0.100D-08
  Differentiating once with respect to electric field.
    with respect to dipole field.
  Differentiating once with respect to nuclear coordinates.
Store integrals in memory, NReq= 847198.
  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= 2.80D-16 Conv= 1.00D-12.
Inverted reduced A of dimension 8 with in-core refinement.
End of Minor Frequency-dependent properties file 721 does not exist.
***** Axes restored to original set *****
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal Forces: Max 0.000221616 RMS 0.000221616
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= 9.25D-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 -0.07079.
Iteration 1 RMS(Cart)= 0.00058099 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 0.00082 0.00000 0.00082 2.24989

Item Value Threshold Converged?
Maximum Force 0.000222 0.000450 YES
RMS Force 0.000222 0.000300 YES
Maximum Displacement 0.000411 0.001800 YES
RMS Displacement 0.000581 0.001200 YES
Predicted change in Energy=-9.145683D-08
Optimization completed.
-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
<th>Value</th>
<th>Derivative Info.</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>R(1,2)</td>
<td>1.1902</td>
<td>-DE/DX = 0.0002</td>
</tr>
</tbody>
</table>

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Input orientation:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms) X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
</table>
Stoichiometry: BH
Framework group: C*V[C*(HB)]
Deg. of freedom: 1
Full point group: C*V Noop 4
Largest Abelian subgroup: C2V Noop 4
Largest concise Abelian subgroup: C1 Noop 1

Standard orientation:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>0</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.198360</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0</td>
<td>0.000000</td>
<td>0.000000</td>
<td>-0.991798</td>
</tr>
</tbody>
</table>

Rotational constants (GHZ): 0.000000 386.4235872 386.4235872

Population analysis using the SCF density.

Orbital symmetries:
Occupied (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):

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>B</td>
<td>4.673207</td>
<td>0.299536</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>H</td>
<td>0.299536</td>
<td>0.727721</td>
<td></td>
</tr>
</tbody>
</table>

Mulliken atomic charges:

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>B</td>
</tr>
<tr>
<td>2</td>
<td>H</td>
</tr>
</tbody>
</table>

Sum of Mulliken charges= 0.00000
Atomic charges with hydrogens summed into heavy atoms:

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>B</td>
</tr>
<tr>
<td>2</td>
<td>H</td>
</tr>
</tbody>
</table>
Sum of Mulliken charges = 0.0000
Electronic spatial extent (au): \( <R^{**2}> = 21.7629 \)
Charge = 0.0000 electrons
Dipole moment (field-independent basis, Debye):
\[
X = 0.0000 \quad Y = 0.0000 \quad Z = -2.1064 \quad \text{Tot} = 2.1064
\]
Quadrupole moment (field-independent basis, Debye-Ang):
\[
XX = -6.4995 \quad YY = -6.4995 \quad ZZ = -10.6031
\]
\[
XY = 0.0000 \quad XZ = 0.0000 \quad YZ = 0.0000
\]
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
\[
XX = 1.3678 \quad YY = 1.3678 \quad ZZ = -2.7357
\]
\[
XY = 0.0000 \quad XZ = 0.0000 \quad YZ = 0.0000
\]
Octapole moment (field-independent basis, Debye-Ang**2):
\[
XXX = 0.0000 \quad YYY = 0.0000 \quad ZZZ = -6.6008 \quad XYY = 0.0000
\]
\[
XXY = 0.0000 \quad XXZ = -1.6243 \quad XZZ = 0.0000 \quad YZZ = 0.0000
\]
\[
YYZ = -1.6243 \quad XYZ = 0.0000
\]
Hexadecapole moment (field-independent basis, Debye-Ang**3):
\[
XXXX = -8.6219 \quad YYYY = -8.6219 \quad ZZZZ = -27.1135 \quad XXXY = 0.0000
\]
\[
XXZX = 0.0000 \quad YYYX = 0.0000 \quad YYYYX = 0.0000 \quad ZZZX = 0.0000
\]
\[
ZZZY = 0.0000 \quad XXYY = -2.8740 \quad XXZZ = -5.9598 \quad YYZZ = -5.9598
\]
\[
XXYZ = 0.0000 \quad YYXZ = 0.0000 \quad ZZXY = 0.0000
\]
N-N = 2.223138369423D+00 E-N = -6.245215893605D+01 KE = 2.514250244268D+01
Symmetry A1 KE = 2.514250244268D+01
Symmetry A2 KE = 1.444632664383D-50
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 = 1.19015806

Test job not archived.
1¥1¥GINC-MIRA185¥FOpt¥RSACCI¥D95(d,p)¥B1H1¥MASAHIROY31-Mar-2003¥0¥¥# S
AC-CI(SINGLE=(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-active MOs of D
95**. Initial geometry is the experimental one ¥¥0,1¥B,0.,0,-0.198359
6761¥H,0.,0.,0.9917983806¥¥Version=DEC-AXP-OSF/1-G03RevB.01¥State=1-SG
¥HF=-25.1231312¥RMSD=1.836e-09¥RMSF=1.279e-04¥Dipole=0.,0.,-0.2702436¥
PG=C*V [C*(H1B1)]¥¥@

IT IS BETTER TO THINK YOU ARE HALF DRY THAN TO KNOW YOU
ARE ALL WET. -- SNOOPY

Job cpu time: 0 days 0 hours 0 minutes 15.0 seconds.
File lengths (MBytes): RWF = 114 Int = 0 D2E = 0 Chk = 10 Scr = 28
Initial command:
Warning -- This program may not be used in any manner that competes with the business of Gaussian, Inc. or will provide assistance to any competitor of Gaussian, Inc. The licensee of this program is prohibited from giving any competitor of Gaussian, Inc. access to this program. By using this program, the user acknowledges that Gaussian, Inc. is engaged in the business of creating and licensing software in the field of computational chemistry and represents and warrants to the licensee that it is not a competitor of Gaussian, Inc. and that it will not use this program in any manner prohibited above.

Cite this work as:
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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 03:  DEC-AXP-OSF/1-G03RevB.01 3-Mar-2003
31-Mar-2003

%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, 1/2, 4/1;
3/5 = 8, 7 = 101, 11 = 9, 16 = 1, 125 = 1, 130 = 1, 136 = 2/1, 2, 3;
4/1;
5/5 = 2, 38 = 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, 125 = 1, 130 = 1, 136 = 2/1, 2, 3;
4/5 = 5, 16 = 3/1;
5/5 = 2, 38 = 5/2;
6/7 = 2, 8 = 2, 9 = 2, 10 = 2/1;
7/12 = 7/1, 2, 3, 16;
1/18 = 20/3(-9);
99//99;

-----------------------------------------------
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.

-----------------------------------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
B
H       1       BH

Variables:
    BH            1.232

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
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.

### Input orientation:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms) X</th>
<th>Y</th>
<th>Z</th>
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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:

<table>
<thead>
<tr>
<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms) X</th>
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<th>Z</th>
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<td>-1.026667</td>
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</table>

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 symme try 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)
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. Ebara, 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 ==

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<th>A1</th>
<th>A2</th>
<th>B1</th>
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<tr>
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== Input data for perturbation selection ==

SINGLET STATE
Number of States Singlet = ( 1, 0, 0, 0)
Threshold for perturbation selection of linked operator # LevelThree #
EThresS2 (Lambda_G)= 0.100D-05(au)  EThresR2 (Lambda_E)= 0.100D-06(au)

SINGLET STATE

LINKED OPERATORS FOR SAC:  SYMMETRY = A1  GROUND STATE

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<th>TOTAL</th>
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<tr>
<td>AFTER</td>
<td>16</td>
<td>178</td>
<td>195</td>
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</tbody>
</table>

DEGENERACY IS CONSIDERED FOR SYMMETRY B1  B2

STEP #CIMX#  CI matrix elements

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 (CThresULS2G) 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

<p>| | | | | | | | | | |</p>
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</tbody>
</table>

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)= -0.0818747228 Total energy= -25.2057539683
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
  0 densities were copied.
Do SAC-NV density.
  1 Transform orbital 1 to 19
Compute gradients with respect to orbital rotations.
Evaluate gradients in canonical representation.
CutOGr = 0.100D-08
  Differentiating once with respect to electric field.
  with respect to dipole field.
  Differentiating once with respect to nuclear coordinates.
  Store integrals in memory, NReq= 847198.
  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= 3.00D-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) (SG) (PI) (PI) (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):
\[ X = 0.0000 \quad Y = 0.0000 \quad Z = -1.9774 \quad \text{Tot}= 1.9774 \]
Quadrupole moment (field-independent basis, Debye-Ang):
\[ \begin{align*}
XX &= -6.5397 \\
YY &= -6.5397 \\
ZZ &= -10.6887 \\
XY &= 0.0000 \\
XZ &= 0.0000 \\
YZ &= 0.0000
\end{align*} \]
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
\[ \begin{align*}
XX &= 1.3830 \\
YY &= 1.3830 \\
ZZ &= -2.7660 \\
XY &= 0.0000 \\
XZ &= 0.0000 \\
YZ &= 0.0000
\end{align*} \]
Octapole moment (field-independent basis, Debye-Ang**2):
\[ \begin{align*}
XXX &= 0.0000 \\
YYY &= 0.0000 \\
ZZZ &= -6.3589 \\
XYY &= 0.0000 \\
XXZ &= 0.0000 \\
XZZ &= 0.0000 \\
YYZ &= 0.0000 \\
YZZ &= 0.0000
\end{align*} \]
Hexadecapole moment (field-independent basis, Debye-Ang**3):
\[ \begin{align*}
XXXX &= -8.6681 \\
YYYY &= -8.6681 \\
ZZZZ &= -28.0544 \\
XXYY &= 0.0000 \\
XXZZ &= 0.0000 \\
XYYZ &= 0.0000 \\
YYXX &= 0.0000 \\
YZZX &= 0.0000 \\
XYXZ &= 0.0000 \\
ZZXY &= 0.0000 \\
XYYZ &= 0.0000 \\
XYZ &= 0.0000 \\
XYZZ &= 0.0000 \\

N-N=2.147634773945D+00 \quad E-N=-6.227488917775D+01 \quad KE=2.510485711898D+01
\]
Symmetry A1 KE=2.510485711898D+01
Symmetry A2 KE=0.000000000000D+00
Symmetry B1 KE=0.000000000000D+00
Symmetry B2 KE=0.000000000000D+00
 ***** Axes restored to original set *****

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<th>Center Number</th>
<th>Atomic Number</th>
<th>Forces (Hartrees/Bohr)</th>
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</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.0000000000</td>
</tr>
</tbody>
</table>

Cartesian Forces: Max 0.004656747 RMS 0.002688574

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Internal Forces: Max 0.004656747 RMS 0.004656747
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:
\[ \begin{align*}
R1 \\
R1 &= 0.22470
\end{align*} \]
Eigenvalues --- 0.22470
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
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<tr>
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<th>Old X</th>
<th>-DE/DX</th>
<th>Delta X</th>
<th>Delta X</th>
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Predicted change in Energy=-4.825484D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

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<tr>
<th>Center</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
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</tbody>
</table>

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:

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<th>Center</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
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Rotational constants (GHZ): 0.000000 354.2884318 354.2884318
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 2.1286936587 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:

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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
Spin Multiplicity = 1
Number of Occupied = 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

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== 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

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

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II
### 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

- \( E_{\text{corr}(\text{SAC-NV})} = -0.0819663193 \)
- Total energy = -25.2058069562

Z-vector iteration converged.

Copying SAC-CI densities to excited state density rwf.

- 0 densities were copied.

Do SAC-NV density.

- Transform orbital 1 to 19

Compute gradients with respect to orbital rotations.

Evaluate gradients in canonical representation.

- \( \text{CutOGr} = 0.100D-08 \)
- Differentiating once with respect to electric field.
  - with respect to dipole field.
- Differentiating once with respect to nuclear coordinates.
- 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:**

- \( I_{\text{Opt}} = 1 \)
- \( I_{\text{Iter}} = 1 \)
- \( A_{\text{Max}} = 3.12D-16 \)
- \( \text{Conv} = 1.00D-12 \)

Inverted reduced A of dimension 8 with in-core refinement.

End of Minor Frequency-dependent properties file 721 does not exist.

***** Axes restored to original set *****

---

**Center** | **Atomic Number** | **Forces (Hartrees/Bohr)** | **X** | **Y** | **Z**
---|---|---|---|---|---
1 | 5 | 0.0000000000 | 0.0000000000 | -0.000498087
2 | 1 | 0.0000000000 | 0.0000000000 | 0.000498087

---

**Cartesian Forces:**

- Max 0.000498087 RMS 0.000287571

---

**Berny optimization.**

**Internal Forces:**

- Max 0.000498087 RMS 0.000498087
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:

\[
\begin{array}{cc}
\text{R1} & \text{Eigenvalues} --- 0.20075 \\
\text{R1} & 0.20075 \\
\end{array}
\]

RFO step: Lambda= 0.00000000D+00.
Quartic linear search produced a step of 0.12367.
Iteration 1 RMS(Cart)= 0.00181158 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

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Predicted change in Energy=-6.172605D-07
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

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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:

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Rotational constants (GHZ): 0.0000000 353.5168303 353.5168303
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 = 2.1263743639 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) (SG) (PI) (PI)
- (DLTA) (DLTA) (SG) (PI) (PI) (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: \[ E(RHF) = -25.1238296736 \text{ A.U. after 6 cycles} \]

Convg = 0.8925D-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 = 1 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

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**

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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) = -0.0819779235 Total energy = -25.2058075972
Z-vector iteration converged.
Copying SAC-CI densities to excited state density rwf.
0 densities were copied.
Do SAC-NV density.
  1 Transform orbital 1 to 19
Compute gradients with respect to orbital rotations.
Evaluate gradients in canonical representation.
CutOGr = 0.100D-08
  Differentiating once with respect to electric field.
  with respect to dipole field.
  Differentiating once with respect to nuclear coordinates.
Store integrals in memory, NReq = 847198.
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= 3.00D-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 *****

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</tbody>
</table>

Cartesian Forces: Max 0.000000173 RMS 0.000000100

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Berny optimization.

Internal Forces: Max 0.000000173 RMS 0.000000173

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= 1.04D+00 RLast= 2.56D-03 DXMaxT set to 3.00D-01

The second derivative matrix:

<table>
<thead>
<tr>
<th>R1</th>
</tr>
</thead>
</table>

Eigenvalues --- 0.19448

RFO step: Lambda= 0.00000000D+00.

Quartic linear search produced a step of -0.00034.

Iteration 1 RMS(Cart)= 0.00000062 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 0.000001 0.001200 YES

Predicted change in Energy=-7.657447D-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

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Input orientation:
Center | Atomic Number | Atomic Number | Atomic Type | Coordinates (Angstroms) 
--- | --- | --- | --- | --- 
| | | | | 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 Number | Atomic Number | Atomic Type | Coordinates (Angstroms) 
--- | --- | --- | --- | --- 
| | | | | 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  353.5168303  353.5168303

********************************************************************************
Population analysis using the SCF density.
********************************************************************************

Orbital symmetries:
Occupied (SG) (SG) (SG)
Virtual (PI) (PI) (SG) (PI) (SG) (SG) (PI) (PI)
(DLTA) (DLTA) (SG) (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= 0.00000 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  XYY= 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  YYYY= 0.0000  YZZ= 0.0000  ZZZX= 0.0000
  YYYY= 0.0000  XXXY= -2.8942  XXZZ= -6.1708  YYZZ= -6.1708
  XXXY= 0.0000  XXZ= 0.0000  XZZ= 0.0000
N-N= 2.126374363943D+00  E-N= -6.222464831208D+01  KE= 2.509453989671D+01
Symmetry A1 KE= 2.509453989671D+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=1.24431807

Test job not archived.

WHAT, THEN, IS TIME? IF NO ONE ASKS ME, I KNOW WHAT IT IS.
IF I WISH TO EXPLAIN WHAT IT IS TO HIM WHO ASKS ME, I DO NOT KNOW.
-- ST. AUGUSTINE (FIFTH CENTURY)

END OF GUIDE FOR SAC-CI/Gaussian