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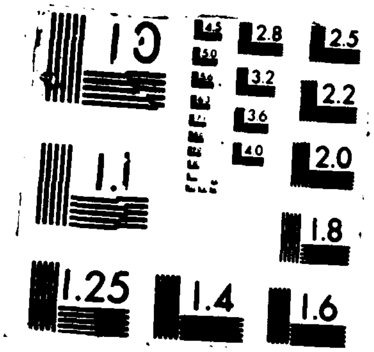
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MATTHEW J. KERPER
Chief, Technical Information Division

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ABSTRACT

The goal of this project is to develop methods for calculating molecular activation energies. The project has been highly successful, as it has resulted in the development of a state of the art quantum chemistry package to do these calculations. This package contains a highly vectorized CI program which appears to be the fastest CI program that is currently in existence. Due to its speed and efficiency, the CI program has the potential for widespread applications in many areas involving molecular energetics. The importance of this program stems from the fact that in molecular energy calculations, the CI method will yield the best possible result that can be obtained for a given basis set. In addition to the CI program, this comprehensive quantum chemistry package also contains state of the art SCF, geometry optimization, and vibrational frequency programs.

I. INTRODUCTION

The goal of this project is to calculate the amount of shocking or jostling that a solid explosive can withstand before detonating. The ultimate objective is to determine, by means of the calculations, how to modify the explosive so that it still retains all of its explosive power but becomes less sensitive to shock. These less sensitive but equally powerful explosives would reduce the number of accidents that occur among personnel involved in handling, storing, transporting, and using the explosives.

The detonation process is complicated and involves many factors, including "hot spots", propagation of acoustic or detonation waves, interaction (or scattering) between detonation waves and explosive molecules, etc. However, the key factor in an explosive's sensitivity to shock is the activation energy of the molecules that make up the explosive. When an explosive receives a shock, the energy of the molecules contained in the explosive is increased. In the region of the shock, if the energy of a sufficient number of molecules is raised above the activation energy, then the detonation begins. Thus if one can increase the activation energy, a bigger shock will be required for detonation and the explosive will be safer to handle. Therefore the first step in the study of detonations is to determine accurate values for the activation energy of the explosive molecules.

One can determine the activation energy of an explosive molecule by calculating the total energy of the molecule as a function of a reaction coordinate such as a bond length or bond angle. At the value of the reaction coordinate where the total energy goes through a maximum, dissociation, or detonation, occurs, and the activation energy is the difference between this maximum total energy and the total energy of the molecule in its equilibrium state.

In order for these calculated activation energies to be sufficiently accurate to be useful in experimental and developmental work, it is essential that electron correlation effects be included in the calculations, as electron correlation plays a very crucial role in molecular energetics. We have included correlation effects by means of the CI method, which has the capability of yielding the best possible results that can be obtained for a given basis set.

Very substantial progress has been achieved in the CI method, and as a result this project is considered to be highly successful. Specifically, we have developed a state of the art quantum chemistry package that contains what appears to be the fastest CI program that is currently in existence. This highly vectorized CI program has the potential for widespread applications in many areas involving molecular energetics.

II. CRAY QUANTUM CHEMISTRY PACKAGE

The configuration interaction (CI) method is probably the best known and most widely recognized procedure for including electron correlation effects in molecular energy calculations. If carried to completion, the CI calculation will yield the best possible result that can be obtained for a given basis set. A complete or full CI calculation is one which includes all of the possible excitations of electrons from occupied to empty states. In practice it is often not necessary to carry the CI all the way to completion, but rather to converge the CI to whatever degree of accuracy one desires for the molecular energies. A converged CI usually requires at least all single and double excitations and sometimes all triple and quadruple excitations as well. Since the number of double, triple and quadruple excitations can be quite large for some energetic molecules of interest, the CI calculation can be very time-consuming, and therefore one needs very fast CI programs and very fast computers in order to make the calculations feasible. We have obtained Dr. Henry F. Schaefer's CI programs[1-10], which are generally considered to be the best and fastest CI programs in the world. In addition to their speed, Dr. Schaefer's programs have the capability of handling very large numbers of excitations while yielding exact results for the CI energies. This last feature is particularly important since many other CI programs are severely limited in the number of excitations that can be included in the CI calculation.

We have made very substantial progress in this area by converting the entire Schaefer CI package to the CRAY. Not only are these CI programs running on the CRAY, but also they have been <u>vectorized</u> to take full advantage of the multi-processing capability of the CRAY. As a result of this vectorization, these CI programs are now running very fast and efficiently. Test calculations indicate that these vectorized CI programs, when run on the CRAY, are probably the fastest CI programs that are currently in existence.

In addition to the CI programs, our quantum chemistry package contains a state of the art SCF program that will handle large molecules and large basis sets, and will perform both RHF and ROHF calculations on these large systems with d functions included in the basis set. The package also contains a state of the art geometry optimization program that has the same capacity for handling large molecules as does the SCF program, and that works well for ROHF high spin states as well as singlet states. This program is probably the best geometry optimizer that is currently available. In addition, our quantum chemistry package has a new state of the art vibrational frequency program that yields highly accurate values for molecular vibrational spectra.

III. ACTIVATION ENERGY OF FLUORINE AZIDE

Our CRAY quantum chemistry package was used to perform extensive CI calculations of the activation energy (barrier height) of fluorine azide (FN_3), which is a highly energetic molecule. We are grateful to Dr. Harvey Michaels for a useful discussion in which he provided us with the theoretical geometry of FN_3 in its singlet ground state. Using this information as a guide, we optimized the geometry of the FN_3 singlet at the SCF level by using the Gaussian 82 program[11] and the 6-31G* basis set, and were able to exactly reproduce Dr. Michaels' results. This ground state geometry for FN_3 is shown in Figure 1. The values of the bond lengths and bcnd angles are given in the first line of Table I. As shown by the figure, the ground state FN_3 molecule is planar with the three nitrogens being nearly linear. Having verified that Gaussian 82 works well in geometry optimizations for the FN_3 singlet, we then successively increased the central bond length and optimized the other two bond lengths and the two bond angles at each step of the way. As expected, the optimization calculations show that as the central bond is stretched, the N-F separation decreases, approaching its value for a free NF radical in the closed shell singlet state. The other N-N distance also approaches its value for a free N_2 molecule in the singlet ground state. An interesting feature of the central bond stretching is that the FN_3 molecule becomes more bent as the central bond length is inceased, as indicated by the decreasing value of the N-N-N angle. The stretching of the central bond was continued until the total energy went through a maximum and began to decrease. All of the above geometry optimization calculations were done at the SCF level using the 6-31G* basis set. The FN_3 optimized geometry and SCF total energy at each value of the central bond length are given in Table I. As shown by the table, the SCF calculations give a maximum in the total energy curve at an N_2-NF separation

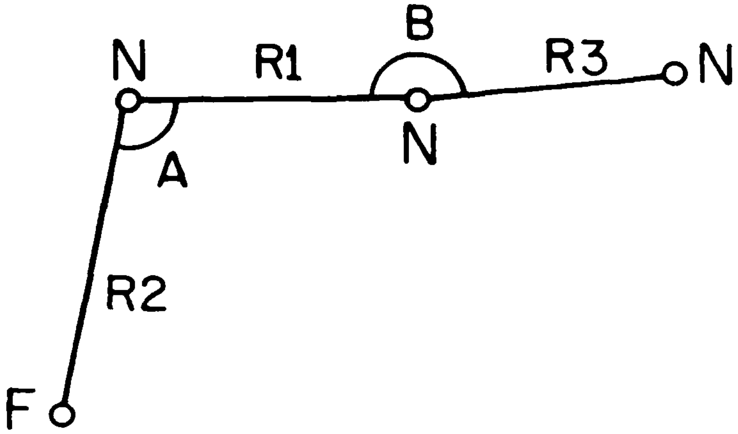

Figure 1. FN_3 ground state geometry.

R1	R2	R3	A	B	SCF
1.2536	1.3819	1.0995	101.33°	173.99°	-262.6024876
⋮					
1.55	1.3677	1.0781	100.20°	170.63°	-262.5854495
1.59	1.3614	1.0773	100.16°	169.85°	-262.5851082
1.63	1.3549	1.0770	100.23°	168.91°	-262.5854492
1.67	1.3480	1.0767	100.38°	167.92°	-262.5863640
1.71	1.3411	1.0766	100.56°	166.72°	-262.5877346
1.75	1.3349	1.0766	100.53°	166.65°	-262.5894411
1.79	1.3280	1.0767	101.02°	164.08°	-262.5913908
1.83	1.3222	1.0768	101.24°	162.68°	-262.5934783
1.87	1.3169	1.0769	101.46°	161.34°	-262.5956300

Table I. Optimized geometry and SCF total energy of the FN_3 singlet for fixed values of the central bond length R1. The top line gives the optimized equilibrium geometry of the FN_3 singlet ground state. The geometry optimizations were done at the SCF level using the 6-31G* basis set. The bond lengths and angles are defined in Figure 1. The SCF total energies, which are given in the last column, are in Hartrees, and the bond lengths are in Angstroms.

	SCF
N_2	-108.9439495
NF(a)	-153.7029725
NF(b)	-153.6734332

Table II. SCF total energy of the singlet ground state of N_2 and the open and closed shell singlet excited states of NF, labeled NF(a) and NF(b) respectively. The SCF calculations were done using the 6-31G* basis set. Energies are in Hartrees.

R1	SCF	CISD	CISD+DC
1.2536	-262.6024876	-263.1860553	-263.2636103
.			
.			
.			
1.55	-262.5854495		
1.59	-262.5851082	-263.1567073	-263.2334369
1.63	-262.5854492	-263.1550073	-263.2312606
1.67	-262.5863640	-263.1540325	-263.2298197
1.71	-262.5877346	-263.1536820	-263.2290301
1.75	-262.5894411	-263.1538678	-263.2288214
1.79	-262.5913908	-263.1544530	-263.2290555
1.83	-262.5934783	-263.1553541	-263.2296515
1.87	-262.5956300	-263.1564707	-263.2305061

Table III. SCF, CISD, and CISD+DC total energies of the FN_3 singlet for values of the central bond length R1. The CISD and CISD+DC calculations were done using the geometries that were optimized at the SCF level. R1 is in Angstroms and the energies are in Hartrees.

of approximately 1.59 Å, and a barrier height of .47 eV.

We also performed SCF calculations on the FN_3 decomposition products, which include the N_2 singlet ground state and the two NF singlet excited states. The lower of these NF excited states, which is an open shell singlet, will be labeled NF(a) while the upper one, which is a closed shell singlet, will be labeled NF(b). Table II gives the SCF total energies of these states. According to the SCF results, the separated products NF(b)+N_2 lie .41 eV below the FN_3 singlet ground state, while the NF(b) and NF(a) states are separated by .80 eV.

After the SCF calculations were completed, we employed the CRAY CI package to perform CI calculations on FN_3, using the geometries that were optimized at the SCF level. The CI calculations included all single and double excitations (CISD) and employed the 6-31G* basis set. No frozen core was used in these calculations; all of the FN_3 electrons were included in the CI, giving a total of 228,826 configurations for the FN_3 singlet. The Davidson correction (DC) for quadruple excitations was also computed and added to the CISD energies. The results of these calculations for FN_3 are shown in Table III. According to the table, the CISD calculation gives a total energy maximum at 1.71 Å and a barrier height of .88 eV, while the CISD+DC calculation gives a maximum at 1.75 Å and a barrier height of .95 eV. These results can be compared with the corresponding SCF values of 1.59 Å and .47 eV. Thus the CISD and CISD+DC correlation treatments produce a major change in the barrier height, causing it to increase to approximately twice its value at the SCF level. This shows that CI is essential to an accurate description of the FN_3 decomposition process.

IV. CI FORMALISM

We now give a brief description of the CI formalism. The CI method[12,13] is used to solve the electronic Schroedinger equation:

$$H\Psi = E\Psi \tag{1}$$

where the Hamiltonian H, in atomic units, is given by

$$H = V_{NN} + \sum_{\mu} h_{\mu} + \sum_{\mu<\nu} g_{\mu\nu} \tag{2}$$

$$V_{NN} = \sum_{A<B} \frac{Z_A Z_B}{r_{AB}} \tag{3}$$

$$h_{\mu} = -\nabla_{\mu}^{2} - \sum_{A} \frac{Z_A}{r_{A\mu}} \tag{4}$$

$$g_{\mu\nu} = \frac{1}{r_{\mu\nu}} \quad . \tag{5}$$

Here the upper-case Latin subscripts represent the nuclei, the lower-case Greek subscripts represent the electrons, the Z's are atomic numbers, and the r's (r_{AB}, $r_{A\mu}$, $r_{\mu\nu}$) are the distances between the particles. The V_{NN} term is the total nuclear repulsion energy.

In order to solve the Schroedinger equation, we write the wave function Ψ as a linear combination of symmetry adapted configuration functions Φ_S:

$$\Psi = \sum_{S} C_S \Phi_S \tag{6}$$

where the Φ_S's are linear combinations of Slater determinants. In a CI calculation, one need include only configurations of the same symmetry as the particular electronic state being investigated (the reference state), since Hamiltonian matrix elements between configurations of different symmetry are zero. Hence the configuration functions are chosen to have the symmetry of the reference state. Since the total number of configurations of all symmetries can be very large, the symmetry adaptation of the configuration functions greatly reduces the size of the Hamiltonian matrix and simplifies the calculation.

The coefficients c_s are chosen to minimize the energy

$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{7}$$

according to the variation principle. The variation principle ensures that the lowest calculated energy is an upper bound for the exact lowest eigenvalue of H (i.e., the exact ground state energy). It also ensures that the lowest calculated energy for each symmetry is an upper bound to the exact lowest eigenvalue of that particular symmetry. Thus if one is investigating an excited state which is the lowest of a particular symmetry type, one need not include any lower states in the same calculation.

Application of the variation principle leads to the well-known eigenvalue equation

$$\sum_t [H_{st}-ES_{st}]c_t = 0 \tag{8}$$

which is solved, by standard techniques, for the eigenvalues E and coefficients c_t. In the above equation, H_{st} and S_{st} are the Hamiltonian and overlap matrix elements, respectively, and are given by

$$H_{st} = \langle\Phi_s|H|\Phi_t\rangle \tag{9}$$

$$S_{st} = \langle\Phi_s|\Phi_t\rangle \quad . \tag{10}$$

The main computational step in a CI calculation is the evaluation of the Hamiltonian matrix elements H_{st}.

In order to construct the configuration functions and evaluate the matrix elements, one chooses a set of atomic basis functions χ_p. One then writes the atomic orbitals ϕ_i as a linear combination of the basis functions

$$\phi_i = \sum_p \chi_p U_{pi} \tag{11}$$

where the coefficients U_{pi} are determined by an SCF (self-consistent field) or similar calculation. The evaluation of the Hamiltonian matrix elements is greatly simplified if one chooses the atomic orbitals ϕ_i to be orthonormal. The Hamiltonian matrix elements are then given by

$$H_{st} = \sum_{ij} a^{st}_{ij} h_{ij} + \sum_{ijk\ell} b^{st}_{ijk\ell} g_{ijk\ell} \tag{12}$$

where

$$h_{ij} = \langle\phi_i(\vec{r}_1)|h_1|\phi_j(\vec{r}_1)\rangle \tag{13}$$

$$g_{ijk\ell} = \langle\phi_i(\vec{r}_1)\phi_k(\vec{r}_2)|g_{12}|\phi_j(\vec{r}_1)\phi_\ell(\vec{r}_2)\rangle \tag{14}$$

and the coefficients a^{st}_{ij} and $b^{st}_{ijk\ell}$ are determined by a projective reduction calculation[14]. The integrals h_{ij} and $g_{ijk\ell}$, which are called orbital integrals, can be obtained from analogous basis set integrals, $\bar{h}_{ij}$ and $\bar{g}_{ijk\ell}$, by the transformation

$$h_{ij} = \sum_{pq} U^*_{pi} U_{qj} \bar{h}_{pq} \tag{15}$$

$$g_{ijk\ell} = \sum_{pqrs} U^*_{pi} U_{qj} U^*_{rk} U_{s\ell} \bar{g}_{pqrs} \tag{16}$$

where

$$\bar{h}_{pq} = \langle\chi_p(\vec{r}_1)|h_1|\chi_q(\vec{r}_1)\rangle \tag{17}$$

$$\tilde{g}_{pqrs} = \langle x_p(\vec{r}_1)x_r(\vec{r}_2)|g_{12}|x_q(\vec{r}_1)x_s(\vec{r}_2)\rangle \quad . \tag{18}$$

The transformation of the two-electron integrals, Eq. (16), can be quite time-consuming and must therefore be handled efficiently.

To summarize, the major computational steps in a CI calculation are the following:

1) Choose a basis set and compute the basis set integrals
2) Determine the orbitals by means of an SCF calculation
3) Transform the basis set integrals to orbital integrals
4) Choose and construct a set of symmetry adapted configuration functions for the electronic state that is being investigated
5) Calculate the Hamiltonian matrix elements with respect to the configuration functions
6) Compute the lowest eigenvalue(s) and eigenvector(s) of the Hamiltonian matrix

As mentioned previously, a full CI calculation (one in which all the configurations of a particular symmetry are included) yields the best possible total energy that can be computed for a given set of basis functions x_p.

V. USER MANUAL

This manual describes the input to the programs in the CRAY Quantum Chemistry Package. These programs provide the capability of performing restricted Hartree-Fock (RHF) closed shell SCF calculations, RHF open shell (ROHF) SCF calculations, CI calculations, geometry optimizations at the RHF and ROHF levels of SCF theory, and harmonic vibrational frequency calculations at the RHF and ROHF levels.

Programs in this package are limited to molecules whose geometric symmetry belongs to an Abelian point group, i.e., to D_{2h} and subgroups. However, it is always possible to employ less symmetry than a molecule actually posseses. For example, planar CH_3 (D_{3h} symmetry) may be run in C_{2v} point group symmetry; pyramidal CH_3 (C_{3v}) may be run in C_s symmetry. In this way, any molecule may be studied.

Most of the programs contain no fixed dimensions except the size of available memory, which is a machine dependent parameter. By increasing this dimension, one may apply these methods to increasingly larger systems.

OVERVIEW

The SCF, CI, geometry optimization, and force constant evaluation procedures consist of several discreet programs, as contrasted with one huge program module. Each of these programs is summarized below.

INPUT

Program INPUT takes a simple formatted input deck and generates an unformatted direct access file, FTN010. This is a master data file containing such information as the basis set, the AO-SO transformation matrix, and the atomic charges. INPUT need be run only once for a given system.

INTS

This program generates integrals over symmetry-adapted atomic-centered Gaussian basis functions. These include the one-electron (S, T, V) integrals, as well as the two-electron terms, $<\mu\nu|\lambda\sigma>$.

SCF

The SCF program solves the Hartree-Fock-Roothan equations for the self-consistent-field energy and MO coefficients. The MO coefficients, or SCF vector, are stored on the master file, FTN010.

DRT

This program generates the distinct row table (DRT) which is necessary for the graphical unitary group approach (GUGA) configuration interaction (CI) calculation. Information contained in the DRT is also required for the vibrational frequency calculation.

TRANS

This program performs the transformation of integrals from the atomic-orbital to the molecular-orbital basis using the SCF vector.

CISORT

Program CISORT creates the 3 and 4-external element supermatrices for the GUGA CI program.

CI

This program performs CI calculations using the GUGA method.

AODER

Program AODER evaluates the first and second derivatives of the AO integrals, with respect to atomic displacements. The derivative integrals are multiplied by the appropriate density matrix element to yield the atomic-orbital contribution to the energy gradients.

CPHF

Solution of the coupled-perturbed Hartree-Fock equations is performed by this program. The first-order changes in the SCF coefficients are required for an SCF force constant evaluation.

OPTIM

Given an energy gradient (at any level of theory) OPTIM updates the molecular geometry in the direction of the energy minimum. When the energy gradient falls below an indicated threshold, OPTIM terminates the job.

NORMCO

Given a force constant matrix, this routine performs the diagonalization in mass weighted coordinates, yielding the harmonic vibrational frequencies and the normal modes.

INPUT PARAMETERS

Input to each program comes from both a formatted input deck (unit 5) and an unformatted, direct-access file (FTN010), which is generated by program INPUT. Each program rewinds unit 5 and searches for a 10 character flag which indicates the start of data for that particular program. This allows the input to the various programs to be entered in any order. Unrecognized flags are ignored and may be used to "comment" the input deck. If input to a program is missing, it will result in an abort, or in the selection of default values, if possible.

Program INPUT

It is the function of INPUT to generate the unformatted, direct-access file FTN010, which is read by all subsequent programs. The input to INPUT is designed to be compatible with the HONDO program (Dupuis, King, Rys., J. Chem. Phys., <u>65</u>, 111, 1976). However, not all the HONDO parameters are required here. Hence, a number of dummy parametrs must be entered, for compatibility. The following input description is taken from the comment cards in the HONDO program.

```
-----------------------------------------------------------
-0-    FLAG         # INPUT ##
                    START OF INPUT FOR INPUT
-----------------------------------------------------------
-1-    TITLE        FORMAT(10A8)
-----------------------------------------------------------
-2-
TIMLIM,NPRINT,ITOL,ICUT  FORMAT(F10.0,3I3)

OPTIONS FOR THE JOB

       --- TIMLIM = INTERNAL TIME LIMIT TO STOP THE JOB.
                    NOT USED HERE.
       --- NPRINT =  0  ... NORMAL PRINTING
                  =  1  ... EXTRA PRINTING FOR BASIS SET+SYMMETRY
                  =  2  ... EXTRA PRINTING FOR MO GUESS ROUTINES
                  =  3  ... PRINT OUT 1E-INTEGRALS
                  =  4  ... PRINT OUT 2E-INTEGRALS
                  =  5  ... PRINT OUT SCF DATA FOR EACH CYCLE
                  =  6  ... LIMITED PRINT FOR TSO (72 CHAR./LINE)
                  =  7  ... PUNCH OUT BASIS SET INPUT DATA + MO'S
       --- ITOL   : PRODUCTS OF PRIMITIVES WHOSE
                   PREEXPONENTIAL FACTOR EXP(-G) IS LESS
                   THAN 10.0**(-ITOL) ARE SKIPPED.
                   DEFAULT VALUE : 10.0**(-9)
       --- ICUT   = INTEGRALS LESS THAN 10.0**(-ICUT) IN
                   ABSOLUTE VALUE ARE NOT STORED ON THE
                   INTEGRAL FILE.
                   DEFAULT VALUE : 10.0**(-9)
----------------------------------------------------------
-3- SCHOENFLIES SYMBOL OF THE SYMMETRY POINT GROUP.
    PROGRAM IS LIMITED TO D2H AND SUBGROUPS.
        FORMAT(A5,I5)
POSSIBLE SYMBOLS:  'C1        '
                   'CS        '
                   'CI        '
                   'CNH      I'  I =ORDER OF PRINCIPAL AXIS
                   'CNV      I'
                   'DNH      I'
```

```
----------------------------------------------------------
-4- ORIENTATION OF LOCAL SYMMETRY FRAME
    X1, Y1, Z1, X2, Y2, Z2   FORMAT(6F10.5)
     POINT 1 = (X1,Y1,Z1)    POINT 2 = (X2,Y2,Z2)   TWO DISTINCT POINTS
     USE CARDS 4 AND 5 TO SPECIFY NONSTANDARD ORIENTATION OF
     SYMMETRY ELEMENTS.
     DEFAULT OPTION IS TO LET SYMMETRY FRAME COINCIDE WITH MASTER FRAME.
     TO ELECT DEFAULT OPTION FOR ANY GROUP OTHER THAN C1 LEAVE CARD 4
     BLANK, AND OMIT CARD 5.

     GROUP: SYMMETRY ELEMENTS WITH RESPECT TO LOCAL X,Y,Z FRAME:

     C1     NO SYMMETRY. OMIT CARDS 4 AND 5.
     CS     REFLECTION PLANE = (X,Y)
     CI     CENTER OF INVERSION IS ORIGIN, X=Y=Z=0
     CNH    N-FOLD AXIS = Z, SIGMA-H PLANE = (X,Y)
     CNV    N-FOLD AXIS = Z, SIGMA-V PLANE = (X,Z)
     DNH    N-FOLD AXIS = Z, 2-FOLD AXIS = X, SIGMA-H PLANE = (X,Y)

     MEANING OF POINTS 1 AND 2:
     FOR C1 GROUP, NO CARDS 4 OR 5, GO TO CARD -6-.
     FOR CS GROUP, ANY TWO POINTS IN THE SYMMETRY PLANE.
     FOR CI GROUP, POINT 1 = CENTER OF INVERTION.  (IGNORE POINT 2)
     FOR ALL OTHER GROUPS POINTS 1 AND 2 MAY BE ANY TWO POINTS ON
     LOCAL Z AXIS. (SEE TABLE ABOVE)
--------------------------------------------------------------------
-5-  ORIENTATION OF SYMMETRY FRAME CONTINUED.
            X3, Y3, Z3, DIRECTIONAL PARAMETER    FORMAT(3F10.5,A8)
     POINT 3 = (X3,Y3,Z3)     MUST NOT BE COLINEAR WITH POINTS
                              1 AND 2 ON CARD 4.
     OMIT CARD 5 IF DEFAULT OPTION IS ELECTED ON CARD 4.

     FOR C1 GROUP, OMIT CARD 5.
     FOR CS GROUP, POINT 3 = ANY POINT IN SYM PLANE. IGNORE PARAMETER.
     FOR CI GROUP, OMIT CARD 5.
     FOR OTHER GROUPS, INPUT POINT 3 AND DIRECTIONAL PARAMETER.
     POSSIBLE VALUES OF DIRECTIONAL PARAMETER:
          'PARALLEL'  POINT 3 LIES ON LOCAL X AXIS. (DEFAULT VALUE)
          'NORMAL  '  POINT 3 LIES ON LOCAL Y AXIS.

     COMMENT: THE MOST COMMON USE OF THE 'NORMAL  ' OPTION IS WITH
              DNH WITH ODD N, E.G. STAGGERED ETHANE.  THEN THE LOCAL
              PLANE IS A SIGMA-V PLANE NORMAL TO THE X AXIS.
----------------------------------------------------------
-6- CHARGE , MULTIPLICITY ,UNITS.  FORMAT(3I5)

*******  NONE OF THESE PARAMETERS IS USED HERE             ****
*******  CHARGE,  MULTIPLICITY ENTERED LATER;               ****
*******  COORDINATES ARE ALWAYS IN ATOMIC UNITS (BOHRS)     ****

          CHARGE = +1 FOR NH4+, -1 FOR F- ION, FOR EXAMPLE.
          MULTIPLICITY = 1 FOR CLOSED-SHELL MOLECULE.
          IUNIT > 0 FOR ANGSTROMS.
          IUNIT < OR = 0 FOR ATOMIC UNITS.
```

```
---------------------------------------------------------
-7-  FIRST UNIQUE CENTER     FORMAT(2A4,2X,F5.0,3F20.10)
           NAME,ZNUC,X,Y,Z
        NAME = ATOMIC NAME (USED ONLY FOR PRINT OUT).
        ZNUC = NUCLEAR CHARGE.
        X,Y,Z = COORDINATES IN THE MASTER FRAME IN BOHR.
---------------------------------------------------------
-8-  ISHELL, ITYPE, IGAUSS
     FORMAT(I5,1X,A4,I5)
          ISHELL = SHELL NUMBER ON THIS ATOM.
              FOR EACH ATOM, ISHELL TAKES VALUES 1,2,...
          ITYPE  = SHELL TYPE ='   S' FOR S SHELLS
                               '   P' FOR P SHELLS
                               '   D' FOR D SHELLS
          IGAUSS    = NUMBER OF CONTRACTED PRIMITIVES IN SHELL

***  SPECIAL OPTION:
      THE FOLLOWING CODES WILL CAUSE BASIS SETS TO
      BE READ DIRECTLY FROM THE BERKELEY BASIS SET LIBRARY.
      USE THESE IN PLACE OF ISHELL, ITYPR, IGAUSS.

    GET DZ       -  USE HUZINAGA/DUNNING (9S5P/4S2P)  BASIS FOR H-F
                                         (11S7P/6S4P) BASIS AL-CL
    GET DZP      -  AS ABOVE WITH POLARIZATION.
                    ALSO AUGMENTED WACHTERS BASIS FOR SE-ZN.
    GET TZ       -  USE HUZINGA/DUNNING (9S5P/5S3P) BASIS H-F
    GET WACHTERS -  USE WACHTERS BASIS SETS FOR TRANSITION METALS
    GET STO-3G   -  USE STO-3G BASIS (RIPPED OFF FROM HONDO) H-AR

    IT IS POSSIBLE TO MIX "GET" CARDS WITH ORDINARY BASIS SETS
    ON A GIVEN CENTER (SEE EXAMPLES)
---------------------------------------------------------
IF SPECIAL "GET" TYPE BASIS FUNCTION, NO CARD 9. GO BACK TO -8-
-9- IG, A, C1    FORMAT(I5,E15.9,E20.10)
      IG = PRIMITIVE NUMBER IN THE SHELL ISHELL
         FOR EACH SHELL, IG TAKES VALUES 1,2,...,IGAUSS.
       A = GAUSSIAN EXPONENTIAL PARAMETER OF PRIMITIVE
      C1 = CONTRACTION COEFFICIENT
 ..... THERE ARE IGAUSS CARDS, ONE FOR EACH PRIMITIVE OF SHELL.
 ..... THEN DATA FOR THE NEXT SHELL, RETURN TO CARD-8-.
---------------------------------------------------------
-10- A BLANK CARD ENDS LIST OF SHELLS CENTERED ON THIS ATOM.
...... THEN NEXT UNIQUE CENTER. GO BACK TO CARD-7-
---------------------------------------------------------
-11- A BLANK CARD ENDS THE LIST OF THE UNIQUE CENTERS.
---------------------------------------------------------
```

Program INTS

INTS receives all data from file FTN010; no further input is required. However, one may optionally input new geometric coordinates if desired.

```
----------------------------------------------------------
-0-  FLAG  $NEWGEOM     FORMAT(A10)
            START OF NEW GEOMETRY FOR INTS

            if absent coordinates will be read from FTN010
            if present INTS reads the following cards
----------------------------------------------------------
-1-  CHG,X,Y,Z          FORMAT(4F20.10)

            charge, x, y, z, coordinates for I-th atom
            REPEAT FOR ALL ATOMS
            NOTE: While INPUT requires only unique atomic centers,
                  $NEWGEOM requires ALL coordinates
----------------------------------------------------------
```

Program SCF

-0- FLAG   # SCF ####   FORMAT(A10)
START OF SCF INPUT

-1- ALABEL FORMAT(80A1)

-2- IPRCT, ISCF, IOPEN, INFLG, IVECT, IORDER, PRINT, IDEBUG, ISAVE,
ITRAS, MAXNO, ISTO, MICMX, NCOR, IDFIX

PARAMETERS FOR THE SCF CALCULATION   FORMAT(15I4)

IPRCT : NUMBER OF ITERATIONS BEFORE EXTRAPOLATION.
IPRCT=0 MEANS NO EXTRAPOLATION. (RECOMMENDED)

ISCF : SCF IS CONVERGED WHEN RMS CHANGE IN THE DENSITY MATRIX IS < 10**(-ISCF). DEFAULT=6, BUT 9 RECOMMENDED FOR GRADIENT CALCULATIONS.

IOPEN : = 0 FOR CLOSED-SHELL CALCULATION
= 1 FOR OPEN-SHELL RHF CALCULATION

INFLG : = 0 TO GENERATE NEW SCF VECTOR FROM BARE-NUCLEUS GUESS
: = 1 TO READ OLD VECTOR FROM FTN010
** OLD VECTOR MUST EXIST IF INFLG=1 **

IVECT : = 0 RE-ORDER MO'S BY EIGENVALUE
: = -4 DO NOT RE-ORDER VECTOR

IORDER : = 0 USE OLD VECTOR IN PRESENT ORDER
: <> 0 RE-ORDER MO'S AS INDICATED ON NEXT CARDS

PRINT : PRINT OPTION FOR DEBUGGING

IDEBUG : MORE PRINT OPTION FOR DEBUGGING

ISAVE: NOT USED
ITRAS: NOT USED

MAXNO : MAXIMUM NUMBER OF ITERATIONS. DEFAULT=40.

ISTO : 10**(-ISTO) IS THE THRESHOLD FOR DROPPING INTEGRALS IN THE P AND K TAPE CONSTRUCTION. DEFAULT=20.

MICMX : NUMBER OF MICRO-ITERATIONS (NOT ENABLED)

NCOR : UNIT NUMBER TO READ RELATIVISTIC CORE INTEGRALS (NOT ENABLED)

IDFIX : = 0 COMPUTE OPTIMUM DAMPING FACTOR EACH ITERATION
: <> 0 USE INPUT DAMPING FACTOR FOR ALL ITERATIONS
** WHEN CONVERGENCE IS < 10**(-5) DAMPING IS ALWAYS TURNED OFF

-3- IF IORDER = 0 NO CARD -3-; PROCEED TO -4-
IF IORDER = 1 THEN NEW ORDER OF THE MO'S
FORMAT(17I4)
STARTING EACH SYMMETRY BLOCK ON A NEW CARD, GIVE THE NEW
POSITION OF EACH COLUMN OF THE SCF VECTOR. IF NO RE-ORDERING
IS REQUIRED FOR A GIVEN SYMMETRY BLOCK, BUT IORDER=1,
A UNIT MATRIX MUST BE INPUT. (SEE "REORDERING THE SCF VECTOR").

-4- NCLOS, NOPEN FORMAT(2I5)
ONE CARD FOR EACH SYMMETRY BLOCK
NCLOS : NUMBER OF CLOSED-SHELL ORBITALS IN THE SYMMETRY BLOCK
NOPEN : NUMBER OF OPEN-SHELL OBITALS IN THE SYMMETRY BLOCK

** NOTES: "MISSING" SYMMETRY BLOCKS (EG. A_2 OF DZ H_2O) MUST
APPEAR WITH NCLOS=NOPEN=0

SYMMETRY BLOCKS ARE ASSUMED TO BE IN COTTON'S ORDER,
F.A. COTTON, CHEMICAL APPLICATIONS OF GROUP THEORY,
WILEY-INTERSCIENCE, NEW YORK, 1971.

-5- IF IOPEN = 0 NO CARD -5-; PROCEED TO -6-
IF IOPEN = 1 THEN NOP NUMBER OF CARDS, NOP = N*(N+1)/2,
WHERE N = # OF SYMMETRY TYPES WITH OPEN SHELLS

ALPHA, BETA FORMAT(2F20.10)
COUPLING COEFFICIENTS FOR RHF OPEN-SHELL STATES (SEE OHIO STATE
UNIVERSITY THEORETICAL CHEMISTRY GROUP REPORT # 101)
MOST COMMON TYPES ARE:

HIGH SPIN COUPLED ELECTRONS -
ALPHA = 0.0, BETA = -1.0 FOR ALL NOP CARDS

OPEN-SHELL SINGLET WAVEFUNCTION -
(2 UNPAIRED ELECTRONS IN DIFFERENT SYMMETRY BLOCKS)
ALPHA = 0.0 BETA = -1.0 FOR CARD 1
ALPHA = 0.0 BETA = 3.0 FOR CARD 2
ALPHA = 0.0 BETA = -1.0 FOR CARD 3

-7- DAMP, SHIFTL FORMAT(2F20.10)
DAMP : DAMPING FOR ORBITAL CHANGES (0.0 RECOMMENDED)
SHIFTL : LEVEL SHIFT FOR VIRTUAL ORBITALS (1.0 RECOMMENDED)

In the case of gradient calculation, subroutine TFOCK of the SCF program requires additional input.

-0- FLAG # TFOCK ## FORMAT(A10)
START OF TFOCK INPUT (FOR GRADIENTS)

-1- SCFTYP, CALTYP, DERTYPE FORMAT(3A6)

SCFTYP - INDICATES THE TYPE OF FORMALISM USED USED TO
EVALUATE THE GRADIENT
"GRSCF " SHOULD BE USED WITH THIS SET OF PROGRAMS,
WHICH EMPLOY THE GENERAL SCF FORMALISM

```
               "HSOP   " FOR HIGH-SPIN AND
               "CLSCF  " FOR CLOSED-SHELLS MIGHT BE REQUIRED WITH EARLIER
                         VERSIONS OF THE PROGRAMS

      CALTYP - INDICATES THE TYPE OF ENERGY GRADIENT TO BE PERFORMED
               "SCF    " FOR SCF ENERGY GRADIENTS
               "MCSCF  " FOR MCSCF GRADIENTS (NOT ENABLED)
               "CI     " FOR CI GRADIENTS (NOT ENABLED)

      DERTYP - INDICATES THE ORDER OF THE GRADIENT CALCULATION
               "FIRST " FOR 1ST DERIVATIVES
               "SECOND" FOR 2ND DERIVATIVES
-------------------------------------------------------
-2-   IPRINT   FORMAT(I5)
               PRINT OPTION FOR DEBUGGING
-------------------------------------------------------
```

Program DRT

The Distinct Row Table program generates a series of arrays required by the TRANS, CI and CPHF programs.

```
---------------------------------------------------------
-0-    FLAG    # DRT ####      FORMAT(A10)
               START OF INPUT FOR DRT
---------------------------------------------------------
-1-    ALABLE                  FORMAT(80A1)
---------------------------------------------------------
-2-    OPTIONS CARD FOR CI CALCULATION.  FOR SCF DERIVATIVES,
       LEAVE THIS CARD BLANK.

       OPTION(1), OPTION(2)    FORMAT(2I5)

       OPTION(1) - PRINTING OPTION (POWERS OF TWO TO TURN ON INDIVIDUAL ONES)
                    1 PRINT DRT
                    2 PRINT EXTERNAL WEIGHT ARRAYS
                    4 PRINT INTEGRAL POINTER ARRAYS

       OPTION(2) - EXCITATION LEVEL FOR EXCITATIONS INTO VIRTUALS (DEFAULT 2)
---------------------------------------------------------
-3-    NSYM,   NBF             FORMAT(2I5)

       NSYM  -  NUMBER OF ELEMENTS IN THIS POINT GROUP.
                THIS NUMBER MUST INCLUDE "MISSING" SYMMETRY TYPES
                (NSYM=4 FOR DZ H2O, EVEN THOUGH THERE ARE NO A2 ORBITALS)

       NBF -    TOTAL NUMBER OF BASIS FUNCTIONS
---------------------------------------------------------
-4-    ICOUNT, KEY, ISYM       FREE FORMAT

       ICOUNT - REPEAT COUNT FOR NUMBER OF EQUIVALENT
                ORBITALS OF THIS TYPE

       KEY - ORBITAL CODE
             FOR SCF FORCE CONSTANTS
             VALID TYPES ARE:
             DOC - DOUBLY OCCUPIED ORBITAL
             UOC - UNOCCUPIED ORBITAL
             ALP - ALPHA (HIGH SPIN) OCCUPIED ORBITAL
             SPE - SPECIAL ORBITALS DEFINED LATER

             FOR CI ONE MAY ALSO HAVE:
             FZC - FROZEN CORE ORBITAL
             FZV - FROZEN VIRTUAL ORBITAL

        ISYM - NUMBER SPECIFYING THE SYMMETRY TYPE OF THIS ORBITAL.
               VALUES RANGE FROM 1 TO NSYM.

        REPEAT -4- FOR ALL ORBTALS
```

```
-------------------------------------------------------
-5-     SPECIAL CODE          FREE FORMAT
        IF SPE APPEARS AS AN ORBITAL CODE, THE TYPE OF SPECIAL
        ORBITAL MUST BE IDENTIFIED.  CURRENTLY, THE ONLY VALID
        CODE IS:
        OSS
        INDICATING AN OPEN-SHELL SINGLET CALCULATION
-------------------------------------------------------
```

Program TRANS requires no input.

Program CISORT requires no input.

Program CI

```
--------------------------------------------------------
-0-    FLAG        # CI #####       FORMAT(A10)
--------------------------------------------------------
-1-    IGUESS, MXITER, IROOTI, NROOTS       FORMAT(4I5)

       IGUESS = 0, UNIT VECTOR BASED ON LOWEST DIAGONAL ELEMENT
              > 0, READ IGUESS VECTORS FROM FILE 12 TO START.
       MXITER = MAXIMUM ITERATIONS PER ROOT SOUGHT (10 WITH 2 ROOTS
                GIVES 20 TOTAL).
       IROOTI = FIRST ROOT SOUGHT, DEFAULTS TO 1 WITHOUT STARTING
                VECTORS FOR LOWER ROOTS.
       NROOTS = NUMBER OF TOTAL ROOTS TO BE SOUGHT.
--------------------------------------------------------
```

Program AODER

In the absence of input, AODER will default to the same calculation as indicated for TFOCK. Alternatively, the type of calculation may be overridden, and new options specified.

-0- FLAG # NEWDER # FORMAT(A10)
START OF INPUT FOR AODER

-1- CALTYP, DERTYP, IPRINT FORMAT(2A6,I5)

CALTYP, DERTYP - SAME AS FOR TFOCK
IPRINT - PRINT OPTION

-2- NOSYM, INTOUT, INFOUT FORMAT(A5,2I5)

NOSYM - FOR DEBUGGING, IF NOSYM = "NOSYM", DISABLE SYMMETRY IN THE DERIVATIVE EVALUATION.
- ELSE USE AVAILABLE SYMMETRY.
USE NOSYM = "   "
INTOUT - <> 0 WRITE OUT DERIVATIVE INTEGRALS
INFOUT - <> 0 WRITE OUT TWO-ELECTRON CONTRIBUTION TO DERIVATIVE FOCK MATRIX (FOR CPHF):

$$T^{a}_{\mu\nu} = \sum_{\lambda\sigma i} C_{\lambda i} C_{\sigma i} [2(\mu\nu|\lambda\sigma) - (\mu\lambda|\nu\sigma)]$$

Program CPHF

The CPHF program will use default values if no input is found. The input parameters indicated here are optional

```
---------------------------------------------------------
-0-  FLAG       # CPHF ###      FORMAT(A10)
                START OF INPUT FOR CPHF
---------------------------------------------------------
-1-  IPRINT,  ICNVG,  ITOL,  IPASS      FORMAT(4I5)

     IPRINT -   PRINT OPTION FOR DEBUGGING
     ICNVG  -   ITERATIVE SOLUTION TO THE CPHF IS CONVERGED WHEN
                A*U - B < 10**(-ICNVG).  DEFAULT=8.
     ITOL   -   IN THE ITERATIVE SOLUTION TO THE CPHF,  EXPANSION
                VECTORS ARE DROPPED WHEN THE NORM IS < 10**(-ITOL).
                DEFAULT=17.
     IPASS  -   NUMBER OF PASSES ALLOWED IN THE ITERATIVE SOLUTION
                OF THE CPHF EQUATIONS.  DEFAULT=2.
---------------------------------------------------------
-2-  IGOITR           FORMAT(I5)
           = 0  USE DIRECT INVERSION OF A IF POSSIBLE,
                ELSE USE ITERATIVE SOLUTION.
          <> 0 USE ITERATIVE SOLUTION REGARDLESS OF SIZE.
---------------------------------------------------------
```

Program OPTIM requires no input.

Program NORMCO requires no input.

SAMPLE INPUTS

Formaldehyde SCF optimization in an STO-3G basis

```
# INPUT ##
FORMALDEHYDE IN STO-3G BASIS AT EXPERIMENTAL GEOMETRY
     1000.  0 10 10
CNV      2

    0    1    0
OXYGEN       8.      0.000000000000      0.000000000000     -2.286569522107
GET STO-3G

CARBON       6.      0.000000000000      0.000000000000      0.000000000000
GET STO-3G

HYDROGEN     1.      0.000000000000      1.813400809181      1.023872929647
GET STO-3G


# SCF ####
GROUND STATE SCF
   0  10   0   0   0   0   0   0   0 100   0   0   0   0   0   0   0   0
    5    0
    0    0
    1    0
    2    0
        0.0000000000        1.0000000000

# TFOCK ##
GRSCF SCF   FIRST
    0

# NEWDER #
SCF   FIRST     0
XXXXX    0    0
```

A subsequent run to do the $^1A_2$ state arising from a b_2 --> b_1 excitation and employing the old vector, would have the same input, except for the SCF:

```
# SCF ####
EXCITED SINGLET STATE
   0  10   1   1   0   0   0   0   0 100   0   0   0   0   0   0   0   0
    5   0
    0   0
    1   1
    1   1
        0.0000000000        -1.0000000000
        0.0000000000         3.0000000000
        0.0000000000        -1.0000000000
        0.0000000000         1.0000000000
```

The $^3A_2$ state would have the following input:

```
# SCF ####
EXCITED TRIPLET STATE
   0  10   1   1   0   0   0   0   0 100   0   0   0   0   0   0   0   0
    5   0
    0   0
    1   1
    1   1
        0.0000000000        -1.0000000000
        0.0000000000        -1.0000000000
        0.0000000000        -1.0000000000
        0.0000000000         1.0000000000
```

Fluorine Azide CI calculation with 6-31G* basis set

```
# INPUT ##
FN3,C1,6-31G*,INTEGRAL DATA
1000.
C1
   0    1    0
NITROG1    7.        -1.0382783           3.0050059           0.0
   1    S    6
   1     4173.51    0.00183477
   2     627.458    0.0139946
   3     142.902    0.0685866
   4     40.2343    0.232241
   5     12.8202    0.469070
   6     4.39044    0.360455
   2    S    3
   1     11.6264    -0.114961
   2     2.71628    -0.169117
   3     0.772218   1.14585
   3    S    1
   1     0.212031   1.0
   4    P    3
   1     11.6264    0.0675797
   2     2.71628    0.323907
   3     0.772218   0.740895
   5    P    1
   1     0.212031   1.0
   6    D    1
   1     0.8        1.0

NITROG2    7.         0.0                 1.2052621           0.0
   1    S    6
   1     4173.51    0.00183477
   2     627.458    0.0139946
   3     142.902    0.0685866
   4     40.2343    0.232241
   5     12.8202    0.469070
   6     4.39044    0.360455
   2    S    3
   1     11.6264    -0.114961
   2     2.71628    -0.169117
   3     0.772218   1.14585
   3    S    1
   1     0.212031   1.0
   4    P    3
   1     11.6264    0.0675797
   2     2.71628    0.323907
   3     0.772218   0.740895
   5    P    1
   1     0.212031   1.0
   6    D    1
   1     0.8        1.0
```

```
NITROG3    7.         1.3921164           -0.7114274          0.0
    1    S    6
    1      4173.51    0.00183477
    2      627.458    0.0139946
    3      142.902    0.0685866
    4      40.2343    0.232241
    5      12.8202    0.469070
    6      4.39044    0.360455
    2    S    3
    1      11.6264    -0.114961
    2      2.71628    -0.169117
    3      0.772218   1.14585
    3    S    1
    1      0.212031   1.0
    4    P    3
    1      11.6264    0.0675797
    2      2.71628    0.323907
    3      0.772218   0.740895
    5    P    1
    1      0.212031   1.0
    6    D    1
    1      0.8        1.0

FLUORINE   9.         -0.2752066          -2.721322           0.0
    1    S    6
    1      7001.71    0.00181962
    2      1051.37    0.0139161
    3      239.286    0.0684053
    4      67.3974    0.233186
    5      21.5200    0.471267
    6      7.40310    0.356619
    2    S    3
    1      20.8480    -0.108507
    2      4.80831    -0.146452
    3      1.34407    1.12869
    3    S    1
    1      0.358151   1.0
    4    P    3
    1      20.8480    0.0716287
    2      4.80831    0.345912
    3      1.34407    0.722470
    5    P    1
    1      0.358151   1.0
    6    D    1
    1      0.8        1.0


# SCF ####
SCF GROUND STATE FOR FN3
  00   9   0   0   0   0 000   0   0 300   0   0   0   0   0   0
   15    0
                 0.00              1.000
```

```
# DRT ####
DRT GROUND STATE FOR FN3
    0    2
    1   60
15DOC1 45UOC1


# CI #######
    0   40     0     1
```

Formaldehyde SCF force constant calculation in double-zeta basis

```
# INPUT ##
FORMALDEHYDE IN A DZ BASIS AT EXP. GEOM.
     1000.  0 10 10
CNV       2

    0    1    0
OXYGEN         8.        0.000000000000        0.000000000000       -2.286569500000
    1    S    6
    1 .781654000E+04  0.203100000000E-02
    2 .117582000E+04  0.154360000000E-01
    3 .273188000E+03  0.737710000000E-01
    4 .811696000E+02  0.247606000000E+00
    5 .271836000E+02  0.611832000000E+00
    6 .341360000E+01  0.241205000000E+00
    2    S    1
    1 .953220000E+01  0.100000000000E+01
    3    S    1
    1 .939800000E+00  0.100000000000E+01
    4    S    1
    1 .284600000E+00  0.100000000000E+01
    1    P    4
    1 .351832000E+02  0.195800000000E-01
    2 .790400000E+01  0.124189000000E+00
    3 .230510000E+01  0.394727000000E+00
    4 .717100000E+00  0.627375000000E+00
    2    P    1
    1 .213700000E+00  0.100000000000E+01

CARBON         6.        0.000000000000        0.000000000000        0.000000000000
    1    S    6
    1 .423260986E+04  0.202900008298E-02
    2 .634882019E+03  0.155349997804E-01
    3 .146097000E+03  0.754109993577E-01
    4 .424973984E+02  0.257120996714E+00
    5 .141892004E+02  0.596554994583E+00
    6 .196659994E+01  0.242516994476E+00
    2    S    1
    1 .514769983E+01  0.100000000000E+01
    3    S    1
    1 .496199995E+00  0.100000000000E+01
    4    S    1
    1 .153300002E+00  0.100000000000E+01
    1    P    4
    1 .181557007E+02  0.185339991003E-01
    2 .398639989E+01  0.115442000329E+00
    3 .114289999E+01  0.386206001043E+00
    4 .359400004E+00  0.640088975430E+00
    2    P    1
    1 .114600003E+00  0.100000000000E+01
```

```
HYDROGEN      1.       0.000000000000        1.813400800000        1.023872900000
    1     S     3
    1 .192406000E+02  0.328280000000E-01
    2 .289920000E+01  0.231208000000E+00
    3 .653400000E+00  0.817238000000E+00
    2     S     1
    1 .177600000E+00  0.100000000000E+01


# SCF ####
SCF GROUND STATE
   0  10   0   0   0   0   0   0   0 100   0   0   0   0   0   0   0   0
    5     0
    0     0
    1     0
    2     0
         0.0000000000         1.0000000000

# TFOCK ##
GRSCF SCF    SECOND
    0

# NEWDER #
SCF    SECOND     0
XXXXX     0     0

# DRT ####
DRT INPUT

    4    24
5DOC1  9UOC1  1DOC3  3UOC3  2DOC4  4UOC4
```

VI. REFERENCES

1. R. R. Lucchese and H. F. Schaefer III, J. Am. Chem. Soc. 99, 6765 (1977).
2. S. Bell and H. F. Schaefer III, J. Chem. Phys. 67, 5173 (1977).
3. R. R. Lucchese and H. F. Schaefer III, J. Chem. Phys. 68, 769 (1978).
4. R. R. Lucchese, B. R. Brooks, J. H. Meadows, W. C. Swope and H. F. Schaefer III, J. Comp. Phys. 26, 243 (1978).
5. B. R. Brooks and H. F. Schaefer III, Int. J. Quant. Chem. 14, 603 (1978).
6. N. C. Handy, J. D. Goddard and H. F. Schaefer III, J. Chem. Phys. 71, 426 (1979).
7. Y. Yoshioka, J. D. Goddard and H. F. Schaefer III, J. Chem. Phys. 74, 1855 (1981).
8. Y. Osamura, Y. Yamaguchi and H. F. Schaefer III, J. Chem. Phys. 75, 2919 (1981).
9. Y. Osamura, Y. Yamaguchi and H. F. Schaefer III, J. Chem. Phys. 77, 383 (1982).
10. D. J. Fox, Y. Osamura, M. R. Hoffmann, J. F. Gaw, G. Fitzgerald, Y. Yamaguchi and H. F. Schaefer III, Chem. Phys. Lett. 102, 17 (1983).
11. Gaussian 82, Revision H, Carnegie-Mellon University, 1984.
12. H. F. Schaefer III, The Electronic Structure of Atoms and Molecules, (Addison-Wesley, Reading, Mass., 1972).
13. I. Shavitt, in Modern Theoretical Chemistry: Electronic Structure Theory, edited by H. F. Schaefer III, (Plenum Press, New York, 1977), Vol. 3, Chapter 6.
14. S. F. Boys and G. B. Cook, Rev. Mod. Phys. 32, 285 (1960).

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