CHEM409 PChem Lab Home Page - Dr. Pat Owens

PChem Message Board

Email the Professor!! owensp@winthrop.edu

Course Info

CHEM407

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CHEM409

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Useful Tools and References

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Colby's Mol File Convertor

Spartan's User's Guide
NIST Chemistry Webbook
NIST Constant Index

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Other Links

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Chemistry-Physics-Geology
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ACS Div of PChem
UGA's Comp Quantum Chem
WWW Comput Chem

CHEM409, Fall 1998, Dr. Pat Owens

(owensp@winthrop.edu)

Lab Projects Lab Reports Computational Chemistry Grading

Class Times: TBA

Office Hours: SIMS108A - Tuesday and Thursday 8:30-9:30

Text: *Physical Chemistry: Methods, Techniques and Experiments*, Rodney J. Sime.

Outline: This semester you will conduct 7-8 experiments over the course of the semester. Data collection will be conducted in groups of two or three; individual lab reports will be required.

The focus of this semester's lab program will be to utilize various spectroscopic and computational techniques to investigate molecular structure and properties. Many of the experiments will utilize techniques for which there is only one instrument available. Groups will schedule time to collect data at some point during the week when it is not being utilized by other groups or courses.

Lab projects

Here is a tentative list of projects that will be completed this semester. Expect this to be updated as the semester progresses.

1. Spectrum of a Particle in a Box - Exp #34, p.687

The diode array spectrometer will be used to measure absorbance maxima of a series of methine dyes. These will be compared to results expected from a FEMO "particle in a box" model reported in the literature for these compounds. Students will then conduct semi-empirical MO calculations to compare the HOMO-LUMO energies for these dyes.

2. Ab Initio Determination of Ionization Energies for Various Elements

The predicted ionization energy for a series of elements will be calculated using various QM computational techniques. These will be compared with literature values and with computational requirements.

3. Vibration-Rotation Spectra of a Diatomic Molecule

The Nicolet FT-IR spectrometer will be used to measure the rovibrational spectra of HCl. A number of molecular parameters will then be calculated..

4. Determination of Molecular Properties using *ab initio* calculations.

5. Electronic Spectrum of Iodine

The dual-beam UV/Vis spectrometer will be used to measure the spectrum of iodine; from these the dissociation energy and other parameters will be determined.

6. Internal Rotation N,N-dimethylacetamide using Spartan

Students will use Spartan to generate a predicted PE curve as a function of dihedral angle to characterize internal rotational barriers.

7. Internal Rotation rates for N,N-dimethylacetamide.

A Jeol 300MHz NMR with variable temperature probe will be used to evaluation the NMR spectra over a range of temperatures.

8. Viscosity of Solutions of Macromolecules - Exp #14, p.522.

Computational Chemistry

A number of the labs will require computational chemistry calculations involving Hyperchem or Spartan molecular modeling software. A Pchem account has been established on all SG workstations. The account information is:

User: pchem
Password: (see me)

Set up a folder within the Pchem account to save all your files and to partition it from the work of others. Even if someone is using the machine your folder is on, you can remotely access it at any time from any of the other workstations.

Lab Reports

Your goals should be to make your lab reports professional and very much like papers published in peer-reviewed journals. Reports should have these sections:

- Abstract (purpose and experimental method, results, and conclusions)
- Introduction (purpose and theory)
- Experimental Procedures (sufficient detail for someone to repeat the experiment)
- Calculations and Results (organized, show trends, illustrative data & figures, meaningful and well conveyed)
- Discussion and Conclusions (basis for trends, relate to theory, significant conclusions)
- References
- Appendices (organized and tabbed clearly)

Ionization Energy Lab

Dr. O's HF STO3-21G* Output Files

(* indicates STO-3G Calculation)

H							He *
							He+*
Li	Be	B	C	N	O	F	Ne*
Li+	Be+	B+	C+	N+	O+	F+	Ne+*
Na	Mg	Al	Si	P	S	Cl	Ar
Na+	Mg+	Al+	Si+	P+	S+	Cl+	Ar+
K	Ca						
K+	Ca+						

Water *Ab Initio* Lab

You will conduct a number of *ab initio* calculations to better understand the capabilities and limitations of quantum mechanics.

Molecular modeling is a powerful tool which allows property calculation once the true wavefunction is known. Unfortunately, for multi-electron atoms and molecules, Schrodinger's equation cannot be solved and only an approximate wavefunction can be found. The variational principle states that calculated energies from approximate wavefunctions are greater than true energies. Wavefunctions that predict energies closest to experimental energies serve as the best approximations to true wavefunctions.

In approximate wavefunctions, molecular orbitals are represented as sums of "basis functions" which are atomic orbitals centered on the various atoms (most modern *ab initio* methods express each basis function as a sum of Gaussian type orbitals to increase the speed of the calculation). Larger sets of basis functions generally do better at predicting properties, but come with greater computational costs. For large molecules (such as proteins), *ab initio* calculations are not practical and semi-empirical or molecular mechanics methods have to be used. For small molecules, *ab initio* methods are quite practical.

In this lab, calculations for water will use basis sets of increasing sophistication to determine the effect of basis set selection on property prediction and computational requirements.

Larger basis sets involve 1) more Gaussian functions for core or valence shells, 2) multiple sets (e.g. double zeta) of valence basis functions to account for anisotropic (nonspherical) electron distributions, and 3) polarization functions (p-type for H atoms, d-type for other atoms (**notation indicates both types of polarization functions are used, * indicates polarization functions for H atoms). Polarization basis functions allow the electronic charge to be off-center from a nucleus.

1. Using **geometry optimization**, predict the properties of water listed below with each of these five basis sets: STO-3G, STO3-21G*, STO6-31G*, STO6-311G**, and STO6-311G** with MP2 (Note: MP2 is an *ab initio* procedure to correct for the correlation energy which the HF method does not account for). In each case, compare your results with experimental values and with computational requirements (CPU time found under ***display, output*** at end of file).

    a. **Total Energy** (found under the properties menu)
    (Note: The total energy includes all electron-electron repulsions, electron-nucleus attractions, nucleus-nucleus repulsions, and electron kinetic energies. It does not include molecular translational energy, rotational energy, or vibration energy. The experimental total electronic energy of water is -76.481 hartrees. (Levine, *Quantum Chemistry*, p.395).
    b. **Bond angle** (found under the geometry menu)
    c. **Bond distance** (found under the geometry menu)
    d. **Dipole moment** (found under the properties menu)
    e. **Vibrational frequencies** (there are three of these for water) (found under the properties menu, must select Frequency box in *ab initio* setup as option)
    f. **Ionization energy** (use Koopman's theorem) (remember to include PRINTMO as an option)

2. From the STO6-311G** with MP2 calculation, determine the percentage of the correlation energy

that the MP2 calculation corrects for (compare HF, Post HF, and experimental energies).

Water *ab initio* Lab

Dr. O's Output Files

STO-3G	STO3-21G*	STO6-31G*	STO6-311G**	STO6-311G**MP2

HCl Rovibrational Spectral Analysis Lab

In this lab you will measure the rovibrational infrared spectrum of HCl and use spectral information to determine rotational constants, moments of inertias and bond lengths for each of the first two vibrational states of HCl.

1. Measure the infrared spectrum of HCl in the region of 2600-3100 cm^{-1}. This can be accomplished by:
   - Collecting a background spectrum with the gas cell in place.
   - Placing a drop of concentrated HCl in the cell, letting it evaporate for a few minutes before collecting the spectrum.
   - Examining the 2600-3100 cm^{-1} region. HCl infrared absorptions occur there, while water bands are found in other parts of the spectrum.
2. R and P branch transitions are due to energy differences between rovibrational states.

The energy of a particular state (S(v,J)) is due to vibrational and rotational energy contributions:

$$S(v,J) = (v+1/2)\,\nu + B_v\,J\,(J+1)$$

where v and J are vibrational and rotational quantum numbers, B_v is the rotational constant associated with the vibrational level having quantum number v, and ν is the vibrational wavenumber.

An R transition corresponds to a ΔJ of +1, while a P transition denotes a ΔJ = -1 change. Energy expressions for the R and P bands can be found by taking the difference in energies found using the S(v,J) expression. This results in:

$$R(J) = \nu + (B_1 + B_0)\,(J+1) + (B_1 - B_0)\,(J+1)^2$$

$$P(J) = \nu - (B_1 + B_0)\,J + (B_1 - B_0)\,J^2$$

Because of the difference in rotational constants for the first two vibrational levels ($B_1 < B_0$), the P transitions get further apart and the R transitions get closer together as J increases.

3. From a plot of R(J) vs J+1, and a plot of P(J) vs. J; determine ν, B_1, and B_0 using a 2nd order linear regression analysis of the R(J) and the P(J) expressions above. Then calculate the moments of inertia and bond lengths for the first two vibrational states. Finally, calculate the force constant k for HCl.

4. **Note:** Since the highest available resolution available on the FT-IR is 2 cm^{-1}, you will not be able to measure separate bands for HCl^{35} and HCl^{37}.

Iodine Electronic Spectroscopy Lab

In this lab you will measure the visible spectrum of iodine and determine dissociation energies and vibrational frequencies for the ground "X" electronic level (a $^1\Sigma_g$ state) and the "B" excited electronic level (a $^3\Pi_{0u}{}^+$ state). Experiment 31 in the lab text and the Atkins text provide background information.

Electronic Spectroscopy

Transitions between different electronic states have vibrational and rotational energies associated with them. While individual transitions from rotational states cannot be resolved, it is often possible to resolve vibrational transitions in the electronic spectra of gas-phase molecules.

For a given electronic state, the vibrational energy for an anharmonic oscillator is

$$G(\nu)\ (cm^{-1}) = \nu_e\ (v + 1/2) - \nu_e\chi_e\ (v + 1/2)^2 + \nu_e y_e\ (v + 1/2)^3 + ... \qquad (1)$$

For iodine, electronic transitions occur from the low lying vibrational states (v" = 0 primarily) of the X electronic state to a series of excited vibrational states (v') in the B electronic state. Neglecting rotational contributions, the energies (ν) of each transition correspond to differences in electronic and vibrational energies:

$$\nu\ (cm^{-1}) = T_{el} + G(v') - G(v") \qquad (2)$$

where is T_{el} is the energy difference between the potential energy minima of the two electronic states, v' is the quantum number for the vibrational level in the excited electronic state and v" corresponds to the vibrational quantum number of the ground electronic state. Transitions occur from a v" level of the ground electronic state to a v' level of the excited electronic state. Combining (1) and (2) leads to an energy expression for each vibrational peak in the spectrum:

$$\nu\ (cm^{-1}) = T_{el} + \nu_e'(v'+1/2) - \nu_e\chi_e'(v'+1/2)^2 + \nu_e y_e'(v'+1/2)^3 - \nu_e"(v"+1/2) + \nu_e\chi_e"(v"+1/2)^2 - \nu_e y_e"(v"+1/2)^3 \qquad (3)$$

From the set of absorption frequencies of transitions from the v" = 0 level to various v' states, a regression using equation (3) allows a third order fit in terms of (v' + 1/2). From a best fit to (3), the excited state parameters ν_e', $\nu_e\chi_e'$, and $\nu_e y_e'$ are calculated. The lab text reports the wavelengths of transitions from the v"=0 state to several v' states. This information is necessary to identify the specific v' states that correspond to each vibrational peak.

The X state dissociates into two iodine atoms that are each in the $^2P_{3/2}$ state. The B state dissociates into one iodine atom in the $^2P_{3/2}$ state and one iodine atom in an excited $^2P_{1/2}$ state. The $^2P_{1/2}$ state of iodine atoms lies 7603.15 cm^{-1} above the $^2P_{3/2}$ state (Moore, C L. "Atomic Energy Levels, Circular of the National Bureau of Standards, US GPO, Washington, D.C. 1958).

It is possible to calculate the ground state dissociation energy without knowing the specific upper v' states being populated. The vibrational peak spacings on the absorption band provide information on the

difference between adjacent vibrational energy levels of the excited electronic state. As v' increases, these differences decrease, in theory reaching 0 at the dissociation limit.

A quantum number n is used to represent the vibrational level of the excited state. The lowest energy transition in the measured spectrum corresponds to an n=0 value. By plotting the differences in energies between adjacent vibrational peaks vs the quantum number n, a Birge-Sponer extrapolation can be made and plotted to estimate the n corresponding to an energy difference of 0. The area under the curve can be represented by the 1/2 * x-intercept*y-intercept. By adding this area to the energy of the n=0 transition, the difference in energy between the v"=0 (of the X state) and the dissociated B excited electronic state can be calculated. Since you already know the $^2P_{1/2}$ state lies 7603.15 cm^{-1} above the $^2P_{3/2}$ state, you now have sufficient information to calculate the dissociation energy for the X state (drawing an energy diagram will help clarify this).

The dissociation energy of the excited electronic state can also be calculated from a separate Birge-Sponer plot of (v'+1/2) vs. ΔE for adjacent vibrational transitions. In this case the dissociation energy represents the area from v'=0 to the dissociation limit.

Between 555 nm and 565 nm, a series of doublet peaks can be seen (see lab text). The peaks on the long wavelength side originate from the v"=1 vibrational state, those on the short wavelength side from the v"=0 state. At wavelengths below 550 nm, only v"=0 type transitions are observed; above 570 nm, only v"=1 transitions are seen. For the doublet peaks in this region, the v' levels corresponding to the v"=1 peaks are 2 higher than for the corresponding v' levels from the v"=0 peaks on the doublet (e.g. for v'=20, v"=0; the adjacent peak corresponds to v'=22, v"=1).

Using two transitions originating from v"=0 and v"=1 levels with the same upper state (v'), one can calculate the energy difference between the v"=0 and v"=1 levels in the X state. This provides information on the vibrational spacing in the X state and an estimate of $\nu_e"-2\nu_e\chi_e"$ (the spacing between v"=1 and v"=0).

Experimental:

You will measure the visible spectrum of I_2 (g) using a double beam spectrophotometer (the diode array does not have sufficient resolution for this experiment). Place iodine crystals in a quartz cuvette--make sure the cap is on the cuvette.

Set up the instrument to measure from 500-650 nm. Use a slit width of 1 and a scan speed of 20 nm/min.

To generate sufficient vapor, you need to heat the sample compartment so that it stays fairly warm during the experiment. Use the heat gun in the NMR room to do this--heat the sample cuvette holder and the metal around it. Also heat the cuvette prior to placing it in the holder--you should see the violet color of the iodine vapor. BE VERY CAREFUL during this step.

You may wish to measure a small portion of the spectrum initially--e.g. from 500-550 nm. Then go back and collect from 540-650 nm.

Obtain a printout of each spectrum and of the peak locations--make sure the threshold is sufficiently low to detect each peak you observe.

Requirements: Using the normal lab report format, make sure to include the following.

1. Tabulate collected data and identify the quantum numbers v'' and v' associated with each observed transition.

2. Determine the excited state parameters ν_e', $\nu_e\chi_e'$, and $\nu_e y_e'$

3. Determine the Dissociation energy (D_o) of the ground electronic state of iodine.

4. Determine the Dissociation energies (D_e and D_o) of the B electronic state.

5. Draw an energy diagram illustrating the relative energies of the two electronic states and all other calculated energies.

6. Determine the energy difference between the v''=0 and v''=1 levels of the X state. Determine the relative populations expected for these two levels at a temperature of 323 K.

7. Explain why the vibrational peaks have different intensities.

8. Comment on the assumption that molecules are harmonic oscillators. Base your statement on your observations or calculations.

9. Compare the dimensions and vibrational frequencies of excited (B) and ground state (X) iodine molecules.

10. Explain why the spacing between vibrational peaks gets closer as the dissociation limit is approached.

NMR Dynamics Lab - Determination of Transition Barriers and Rotation Rates for N.,N-Dimethylacetamide

N,N-Dimethylacetamide (DMA) is a planar molecular having a large rotational barrier about the amide bond. Because of its similarity to peptide bonding geometry, DMA is often used to model peptide rotational barriers to examine conformational changes which are energetically feasible.

In DMA, the N-methyl groups are magnetically nonequivalent, depending on whether the group is cis or trans to the carbonyl. As a result of DMA's rotational restrictions, protons on the N-methyl groups give rise to two separate NMR peaks (near a δ of 3.0) at room temperature. For higher temperatures, rotation rates increase, causing the two NMR peaks to widen due to shorter lifetimes (quicker exchange) of the two conformers. As temperature is further increased (more rapid rotation), the two peaks merge (at the coalescence temperature). Above the coalescence temperature, the merged peak width decreases as temperature increases. This continues until exchange effects no longer contribute to spectral peak widths.

Line Shape Analysis

Line shape analysis of these observed NMR peak shapes allows determination of rotational rate constants at various temperatures. From the known line shape function for two equivalent exchanging groups, four approximations are commonly used to calculate rate constants under conditions ranging from slow to rapid exchange on the NMR time scale.

1. **Slow Exchange:** Below the coalescence temperature and for NMR temperatures at which the two peaks are well resolved (less than ~20% overlap), the rate constant can be calculated using :

$$k = \pi * (h_e - h_o) \qquad (1)$$

where h_o is the Full Width at Half-Height (FWHH) for peaks showing no exchange effects and h_e is the FWHH for peaks widened from exchange effects.

2. **Intermediate Exchange:** Below the coalescence temperature and for NMR temperatures at which the two peaks overlap significantly (minimum between two peaks at least ~20% of peak intensity), the rate constant can be calculated using:

$$k = \pi * 2^{-1/2} * (\Delta\nu_o^2 - \Delta\nu_e^2)^{1/2} \qquad (2)$$

where $\Delta\nu_o$ and $\Delta\nu_e$ are peak separations (in Hz) for spectra without and with exchange effects respectively.

3. **Coalescence:** At the coalescence temperature, the peaks merge into a flat-topped peak and the rate constant can be found with:

$$k = \Delta\nu_o * \pi / 2^{1/2} \qquad (3)$$

4. **Rapid Exchange:** At temperatures at least 10-15 degrees above the coalescence point, the width of the merged peak may be used to calculate k:

$$k = 0.5 * \pi * \Delta\nu_o^2 * (h_e - h_o)^{-1} \quad (4)$$

Kinetic Models and Thermodynamics

The internal rotation about the amide bond is an equilibirum process. The Eyring absolute rate theory can be used to calculate activation parameters.

The rate constant for the exchange of methyl groups (i.e. for rotation about the amide bond) is:

$$k = \kappa * k_B T / h * \exp(-\Delta G^{\ddagger}/RT) \quad (5)$$

$$k = \kappa * k_B T / h * \exp(\Delta S^{\ddagger}/R) * \exp(-\Delta H^{\ddagger}/RT) \quad (6)$$

where k_B is Boltzmann's constant, h is Planck's constant, κ is the transmission coefficient (the fraction of reactant reaching the transition state that goes on to form product--normally assumed to be one), and $\Delta G^{\ddagger}$, $\Delta H^{\ddagger}$, and $\Delta S^{\ddagger}$ are the free energy of activation, the enthalpy of activation, and the entropy of activation respectively.

From the linear plot of ln(k/T) vs 1/T, the entropy and enthalpy of activation can be calculated:

$$\ln(k/T) = \{\ln(\kappa * k_B / h) + \Delta S^{\ddagger}/R\} - \Delta H^{\ddagger}/R * (1/T) \quad (7)$$

The Arrhenius Equation relates rate constants to activation energies:

$$k = A * \exp(-E_a/RT) \quad (8)$$

where E_a is the activation energy and A is the pre-exponential factor. From a plot of ln (k) vs 1/T, E_a can be calculated.

Requirements

1. Determine the coalesence temperature of DMA by collecting proton NMR spectra at multiple temperatures. Start at room temperature and collect an NMR spectrum every 10 degrees. Collect sufficient spectra to determine T_c within one degree. After T_c has been determined, collect spectra at 10, 15, and 20 degrees above T_c.

2. Use the cursers to find the both peak locations and the peak full-width at half maximum for the downfield peak.

3. Use the appropriate line shape analysis equations listed above to determine rate constants for the measured temperatures.

4. Create Eyring and Arrhenius plots and regressions of your data and calculate $\Delta G^{\ddagger}(298)$, $\Delta H^{\ddagger}$, $\Delta S^{\ddagger}$,

and E_a.

5. Use these literature values for DMA rotation parameters: $\Delta H^{\ddagger}$ = 83.68 kJ/mol, $\Delta S^{\ddagger}$ = 19.6648 J / K-mol, and E_a = 86.1904kJ/mol.

PCHEM Ionization Lab Notes

[Follow Ups] [Post Followup] [Dr. Owens' PChem Message Board] [FAQ]

Posted by Dr. O. on September 20, 1998 at 12:06:56:

1. I have created a web page of my output files for the ionization energy lab. If you need to go back and check if you chose the correct HOMO, you may refer to this. The address is:

http://chemistry.winthrop.edu/owens/results/results.html

I have also put a link to it from the pchem home page.

2. Alpha and beta are the two designations for electron spin.

3. If all electrons are paired, the atom is considered a "closed shell" and the software automatically does a "restricted H-F calculation". What this means is that both alpha and beta spin electrons have the same spatial distribution.

4. If there are any unpaired electrons, an "unrestricted HF (UHF) calculation is done. The alpha and beta electrons can then have different spatial distributions--if they actually do then we would expect them to have different energies (eigenvalues).

5. As you are going through and selecting the HOMO's, please notice the energies for orbitals in partially filled subshells--it should make sense to you if you think about it. By the first test, you should understand this....

6. You can pick the experimental IE's off the NIST webbook. A link to that is on the pchem home page.. It makes things easier if you copy and then paste the values directly into a spreadsheet. You can edit the url by just changing the element letters to speed up looking up different elements. Use the Eval value for the IE.

Hope all this helps--if you have questions, please post them for all to see.

Have a great week!!

Dr. O.

PS I have a list of chem majors on our web page now (first item under

news--if your email address is not listed, please send it to me and I will update it.

Follow Ups:

Post a Followup

Name:

E-Mail:

Subject: Re: PCHEM Ionization Lab Notes

Comments:

: 1. I have created a web page of my output files for the : ionization energy lab. If you need to go back and check : if you chose the correct HOMO, you may refer to this. : The address is: : http://chemistry.winthrop.edu/owens/results/results.html : I have also put a link to it from the pchem home page. : 2. Alpha and beta are the two designations for electron spin. : 3. If all electrons are paired, the atom is considered a : "closed shell" and the software automatically does a :

Optional Link URL:

Link Title:

Optional Image URL:

Submit Follow Up Reset

[Follow Ups] [Post Followup] [Dr. Owens' PChem Message Board] [FAQ]

```
..Running Spartan Pre-Processor

water


SPARTAN AB INITIO PROGRAM: SGI/R5K        Release 5.0.1
  (Job run on newton)

  WATER

  Calculation started: Fri Oct  2 15:27:40 1998

  Run type: Geometry optimization
            Numerical Frequency
  Model: RHF/STO-3G
  Number of shells:   4
     3 S shells
     1 SP shells
  Number of basis functions:   7
  Number of electrons:  10
  Use of molecular symmetry enabled
  Molecular charge:   0
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    H  H1          -0.7804951     0.0000000     0.4562610
    O  O1           0.0000000     0.0000000    -0.1140653
    H  H2           0.7804951     0.0000000     0.4562610

  Point Group = CNV Order =  2 Nsymop =  4
  This system has   2 degrees of freedom
   Coordinates read from pre-optimization

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    H  H1           0.0000000    -0.7804951     0.1901087
    O  O1           0.0000000     0.0000000    -0.3802175
    H  H2           0.0000000     0.7804951     0.1901087

  Initial Hessian option
  Hessian will be taken from archive file


Cycle no:   1   Energy =     -74.9625823 rmsG = 0.0238 rmsD = 0.0383

Cycle no:   2   Energy =     -74.9639106 rmsG = 0.0355 rmsD = 0.0192

Cycle no:   3   Energy =     -74.9658902 rmsG = 0.0017 rmsD = 0.0017

Cycle no:   4   Energy =     -74.9659009 rmsG = 0.0005 rmsD = 0.0002

Cycle no:   5   Energy =     -74.9659012 rmsG = 0.0000 rmsD = 0.0000

WATER
```

Cartesian Coordinates (Angstroms)

Atom	Label	X	Y	Z
H	H1	-0.7580832	0.0000000	0.5086753
O	O1	0.0000000	0.0000000	-0.1271688
H	H2	0.7580832	0.0000000	0.5086753

E(HF) = -74.9659012 a.u.

Closed-Shell Molecular Orbital Coefficients

MO:		1	2	3	4	5
Eigenvalues:		-20.25158	-1.25754	-0.59383	-0.45973	-0.39262
		A1	A1	B2	A1	B1
1 H	1 S	-0.00558	-0.15559	0.44922	0.29512	0.00000
2 O	2 S	0.99422	0.23377	0.00000	0.10404	0.00000
3 O	2 S	0.02585	-0.84446	0.00000	-0.53817	0.00000
4 O	2 PX	0.00000	0.00000	-0.61270	0.00000	0.00000
5 O	2 PY	0.00000	0.00000	0.00000	0.00000	1.00000
6 O	2 PZ	0.00416	-0.12283	0.00000	0.75586	0.00000
7 H	3 S	-0.00558	-0.15559	-0.44922	0.29512	0.00000

MO:		6	7
Eigenvalues:		0.58177	0.69263
		A1	B2
1 H	1 S	0.76914	-0.81463
2 O	2 S	0.12581	0.00000
3 O	2 S	-0.82009	0.00000
4 O	2 PX	0.00000	-0.95978
5 O	2 PY	0.00000	0.00000
6 O	2 PZ	-0.76357	0.00000
7 H	3 S	0.76914	0.81463

Estimating Force Constant Matrix by central-differences

System has approximate symmetry Group: CS Order: 1

Problems determining equivalent atoms symmetry turned off

System has approximate symmetry Group: CNV Order: 2

Problems determining equivalent atoms symmetry turned off

Hessian Estimation Complete

Normal Modes and Vibrational Frequencies (cm-1)

	2170.09			4139.70			4390.71		
	A1			A1			B2		
	X	Y	Z	X	Y	Z	X	Y	Z
1	-0.433	0.000	-0.527	-0.559	0.000	0.408	0.523	0.000	-0.438
2	0.000	0.000	0.264	0.000	0.000	-0.205	-0.262	0.000	0.000
3	0.433	0.000	-0.527	0.559	0.000	0.408	0.523	0.000	0.438

```
   ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  1.19 secs.
  Total Wall time:       0 mins.  1.67 secs.

  Calculation finished: Fri Oct  2 15:27:42 1998

SPARTAN PROPERTIES PACKAGE: SGI/R5K        Release 5.0.1

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -20.25158   -1.25754   -0.59383   -0.45973   -0.39262

                        A1        A1        B1        A1        B2
   1 H   1 S        -0.00558   -0.15559    0.44922    0.29512    0.00000
   2 O   2 S         0.99422    0.23377    0.00000    0.10404    0.00000
   3 O   2 S         0.02585   -0.84446    0.00000   -0.53817    0.00000
   4 O   2 PX        0.00000    0.00000   -0.61270    0.00000    0.00000
   5 O   2 PY        0.00000    0.00000    0.00000    0.00000    1.00000
   6 O   2 PZ        0.00416   -0.12283    0.00000    0.75586    0.00000
   7 H   3 S        -0.00558   -0.15559   -0.44922    0.29512    0.00000

  MO:                   6         7

  Eigenvalues:       0.58177    0.69263

                        A1        B1
   1 H   1 S         0.76914   -0.81463
   2 O   2 S         0.12581    0.00000
   3 O   2 S        -0.82009    0.00000
   4 O   2 PX        0.00000   -0.95978
   5 O   2 PY        0.00000    0.00000
   6 O   2 PZ       -0.76357    0.00000
   7 H   3 S         0.76914    0.81463

  Dipole moment:  X =   0.000000  Y =   0.000000  Z =   1.709223
  Total Dipole:   1.709223 Debye

  Mulliken Population Analysis

    AO  ATOM      Occupancy
    --  ----      ---------

     1     1       0.834750
     2     2       1.997836
     3     2       1.848944
     4     2       1.073062
     5     2       2.000000
     6     2       1.410659
     7     3       0.834750

     Atom    Occupancy      Charge
     ----   -----------  -----------

     H  1     0.834750     0.165250
     O  2     8.330500    -0.330500
     H  3     0.834750     0.165250
```

```
  Total Charge =  0.000000


  Natural Atomic Orbital Populations

  Nao  Atom   Type   Basis  Occupancy
  ---  ----  ------- -----  ---------

    1  H  1  S        MIN    0.817067
    2  O  2  S        MIN    2.000000
    3  O  2  S        MIN    1.772727
    4  O  2  PX       MIN    1.147015
    5  O  2  PY       MIN    2.000000
    6  O  2  PZ       MIN    1.446124
    7  H  3  S        MIN    0.817067

  Total MIN occupancy:  10.000000
  Total RYD occupancy:   0.000000
  Total occupancy:      10.000000


  Natural Atomic Populations and Charges

   Atom    Occupancy     Charge
   ----   -----------  -----------

   H  1     0.817067     0.182933
   O  2     8.365866    -0.365866
   H  3     0.817067     0.182933

  Total Charge =  0.000000

Q-minus(NAO) =  -0.3659
Q-plus(NAO)  =   0.1829


  Mulliken Bond Order Matrix

            1         2

   2     0.96419
   3     0.00850   0.96419


   Atomic Valencies

     Atom      Valency
     ----      -------

     H   1     0.972692
     O   2     1.928388
     H   3     0.972692

  Lowdin Bond Order Matrix

            1         2

   2     0.98637
   3     0.00023   0.98637
```

```
  Atomic Valencies

    Atom      Valency
    ----      -------

    H   1     0.986598
    O   2     1.972745
    H   3     0.986598

 Frequencies and reduced mass in atomic units are:

mode     (cm-1)         AU          mass
   1   -0.5416E-04  -0.1110E-15  -0.1874E+16
   2   -0.3021E-04  -0.3453E-16  -0.9765E+16
   3   -0.1711E-04  -0.1108E-16  -0.2597E+17
   4    0.5845E-13   0.1293E-33   0.1809E+30
   5    0.3999E-12   0.6052E-32   0.3931E+28
   6    0.2172E-04   0.1786E-16   0.9849E+16
   7     2170.       0.1782        1.612
   8     4140.       0.6485       0.8739
   9     4391.       0.7296        1.020

 Zero-point vibrational energy is    15.297 kcal/mol

 Standard Thermodynamic quantities at   298.15 K  and     1.00 atm

 Translational Enthalpy:        0.889 kcal/mol
 Rotational Enthalpy:           0.889 kcal/mol
 Vibrational Enthalpy:         15.297 kcal/mol

 Translational Entropy:        34.608  cal/mol.K
 Rotational Entropy:           10.673  cal/mol.K
 Vibrational Entropy:           0.001  cal/mol.K

 Total Cpu time:   0 mins.  0.04 secs.
```

```
..Running Spartan Pre-Processor

water


SPARTAN AB INITIO PROGRAM: SGI/R5K        Release 5.0.1
  (Job run on newton)

  WATER

  Calculation started: Fri Oct  2 15:24:20 1998

  Run type: Geometry optimization
            Numerical Frequency
  Model: RHF/3-21G(*)
  Number of shells:   7
     5 S shells
     2 SP shells
  Number of basis functions:  13
  Number of electrons:  10
  Use of molecular symmetry enabled
  Molecular charge:   0
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    H  H1          -0.7529642     0.0000000     0.4543509
    O  O1           0.0000000     0.0000000    -0.1135877
    H  H2           0.7529642     0.0000000     0.4543509

  Point Group = CNV Order =  2 Nsymop =  4
  This system has   2 degrees of freedom
   Coordinates read from pre-optimization

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    H  H1           0.0000000    -0.7529642     0.1893129
    O  O1           0.0000000     0.0000000    -0.3786257
    H  H2           0.0000000     0.7529642     0.1893129

  Initial Hessian option
  Hessian will be taken from archive file


Cycle no:   1   Energy =     -75.5846382 rmsG = 0.0152 rmsD = 0.0173

Cycle no:   2   Energy =     -75.5858628 rmsG = 0.0046 rmsD = 0.0063

Cycle no:   3   Energy =     -75.5859553 rmsG = 0.0015 rmsD = 0.0010

Cycle no:   4   Energy =     -75.5859598 rmsG = 0.0000 rmsD = 0.0000

WATER


                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
```

```
   -- --------  ------------ ------------ ------------

   H  H1          -0.7804951     0.0000000     0.4562610
   O  O1           0.0000000     0.0000000    -0.1140653
   H  H2           0.7804951     0.0000000     0.4562610

 E(HF)  =     -75.5859598 a.u.

 Closed-Shell Molecular Orbital Coefficients

 MO:                   1         2         3         4         5

 Eigenvalues:      -20.42721  -1.32096  -0.68554  -0.52982  -0.47723

                       A1        A1        B2        A1        B1
  1 H   1 S         -0.00246   0.11499  -0.23228   0.12773   0.00000
  2 H   1 S         -0.00687   0.02049  -0.18208   0.10711   0.00000
  3 O   2 S         -0.98322  -0.22978   0.00000   0.08575   0.00000
  4 O   2 S         -0.09577   0.21802   0.00000  -0.07998   0.00000
  5 O   2 PX         0.00000   0.00000   0.39589   0.00000   0.00000
  6 O   2 PY         0.00000   0.00000   0.00000   0.00000   0.52105
  7 O   2 PZ        -0.00344   0.07919   0.00000   0.44451   0.00000
  8 O   2 S          0.03769   0.70971   0.00000  -0.39387   0.00000
  9 O   2 PX         0.00000   0.00000   0.36968   0.00000   0.00000
 10 O   2 PY         0.00000   0.00000   0.00000   0.00000   0.63234
 11 O   2 PZ         0.00643   0.08988   0.00000   0.51491   0.00000
 12 H   3 S         -0.00246   0.11499   0.23228   0.12773   0.00000
 13 H   3 S         -0.00687   0.02049   0.18208   0.10711   0.00000

 MO:                   6         7         8         9        10

 Eigenvalues:       0.26107   0.36033   1.20668   1.27663   1.78397

                       A1        B2        B2        A1        B1
  1 H   1 S          0.05259   0.03447  -0.96750   0.97558   0.00000
  2 H   1 S          0.86039   1.15577   0.68159  -0.49918   0.00000
  3 O   2 S          0.11032   0.00000   0.00000   0.06586   0.00000
  4 O   2 S         -0.03614   0.00000   0.00000  -0.09311   0.00000
  5 O   2 PX         0.00000   0.30400  -0.19945   0.00000   0.00000
  6 O   2 PY         0.00000   0.00000   0.00000   0.00000   1.02940
  7 O   2 PZ        -0.20775   0.00000   0.00000  -0.25354   0.00000
  8 O   2 S         -1.04126   0.00000   0.00000  -0.09248   0.00000
  9 O   2 PX         0.00000   0.77790  -0.43752   0.00000   0.00000
 10 O   2 PY         0.00000   0.00000   0.00000   0.00000  -0.96504
 11 O   2 PZ        -0.45842   0.00000   0.00000  -0.28550   0.00000
 12 H   3 S          0.05259  -0.03447   0.96750   0.97558   0.00000
 13 H   3 S          0.86039  -1.15577  -0.68159  -0.49918   0.00000

 MO:                  11        12        13

 Eigenvalues:       1.86333   2.02482   3.10329

                       A1        B2        A1
  1 H   1 S          0.23712   0.16494  -0.26627
  2 H   1 S          0.09256   0.48573  -0.35869
  3 O   2 S          0.04198   0.00000   0.08667
  4 O   2 S         -0.12642   0.00000  -1.63841
  5 O   2 PX         0.00000  -1.06606   0.00000
  6 O   2 PY         0.00000   0.00000   0.00000
  7 O   2 PZ         1.01545   0.00000  -0.15375
  8 O   2 S         -0.15994   0.00000   1.96894
```

```
  9 O   2 PX        0.00000    1.41438    0.00000
 10 O   2 PY        0.00000    0.00000    0.00000
 11 O   2 PZ       -1.13209    0.00000    0.46244
 12 H   3 S         0.23712   -0.16494   -0.26627
 13 H   3 S         0.09256   -0.48573   -0.35869

 Estimating Force Constant Matrix by central-differences


 System has approximate symmetry  Group: CS  Order:   1

 Problems determining equivalent atoms symmetry turned off

 Hessian Estimation Complete

 Normal Modes and Vibrational Frequencies (cm-1)


           1799.16                 3812.24                 3945.41
              A1                      A1                      B2
        X      Y      Z         X      Y      Z         X      Y      Z
  1  -0.376  0.000 -0.564    -0.599  0.000  0.354     0.549  0.000 -0.401
  2   0.000  0.000  0.283     0.000  0.000 -0.178    -0.276  0.000  0.000
  3   0.376  0.000 -0.564     0.599  0.000  0.354     0.549  0.000  0.401



   ** Archive file written to unit 12 **

 Total Cpu time:        0 mins.  2.01 secs.
 Total Wall time:       0 mins.  2.49 secs.

 Calculation finished: Fri Oct  2 15:24:22 1998

SPARTAN PROPERTIES PACKAGE: SGI/R5K        Release 5.0.1

 Closed-Shell Molecular Orbital Coefficients

 MO:                   1         2         3         4         5

 Eigenvalues:     -20.42721   -1.32096   -0.68554   -0.52982   -0.47723

                       A1        A1        B1        A1        B2
  1 H   1 S        -0.00246    0.11499   -0.23228    0.12773    0.00000
  2 H   1 S        -0.00687    0.02049   -0.18208    0.10711    0.00000
  3 O   2 S        -0.98322   -0.22978    0.00000    0.08575    0.00000
  4 O   2 S        -0.09577    0.21802    0.00000   -0.07998    0.00000
  5 O   2 PX        0.00000    0.00000    0.39589    0.00000    0.00000
  6 O   2 PY        0.00000    0.00000    0.00000    0.00000    0.52105
  7 O   2 PZ       -0.00344    0.07919    0.00000    0.44451    0.00000
  8 O   2 S         0.03769    0.70971    0.00000   -0.39387    0.00000
  9 O   2 PX        0.00000    0.00000    0.36968    0.00000    0.00000
 10 O   2 PY        0.00000    0.00000    0.00000    0.00000    0.63234
 11 O   2 PZ        0.00643    0.08988    0.00000    0.51491    0.00000
 12 H   3 S        -0.00246    0.11499    0.23228    0.12773    0.00000
 13 H   3 S        -0.00687    0.02049    0.18208    0.10711    0.00000

 MO:                   6         7         8         9        10

 Eigenvalues:       0.26107    0.36033    1.20668    1.27663    1.78397
```

			A1	B1	B1	A1	B2
1	H	1 S	0.05259	0.03447	-0.96750	0.97558	0.00000
2	H	1 S	0.86039	1.15577	0.68159	-0.49918	0.00000
3	O	2 S	0.11032	0.00000	0.00000	0.06586	0.00000
4	O	2 S	-0.03614	0.00000	0.00000	-0.09311	0.00000
5	O	2 PX	0.00000	0.30400	-0.19945	0.00000	0.00000
6	O	2 PY	0.00000	0.00000	0.00000	0.00000	1.02940
7	O	2 PZ	-0.20775	0.00000	0.00000	-0.25354	0.00000
8	O	2 S	-1.04126	0.00000	0.00000	-0.09248	0.00000
9	O	2 PX	0.00000	0.77790	-0.43752	0.00000	0.00000
10	O	2 PY	0.00000	0.00000	0.00000	0.00000	-0.96504
11	O	2 PZ	-0.45842	0.00000	0.00000	-0.28550	0.00000
12	H	3 S	0.05259	-0.03447	0.96750	0.97558	0.00000
13	H	3 S	0.86039	-1.15577	-0.68159	-0.49918	0.00000

MO:	11	12	13
Eigenvalues:	1.86333	2.02482	3.10329

			A1	B1	A1
1	H	1 S	0.23712	0.16494	-0.26627
2	H	1 S	0.09256	0.48573	-0.35869
3	O	2 S	0.04198	0.00000	0.08667
4	O	2 S	-0.12642	0.00000	-1.63841
5	O	2 PX	0.00000	-1.06606	0.00000
6	O	2 PY	0.00000	0.00000	0.00000
7	O	2 PZ	1.01545	0.00000	-0.15375
8	O	2 S	-0.15994	0.00000	1.96894
9	O	2 PX	0.00000	1.41438	0.00000
10	O	2 PY	0.00000	0.00000	0.00000
11	O	2 PZ	-1.13209	0.00000	0.46244
12	H	3 S	0.23712	-0.16494	-0.26627
13	H	3 S	0.09256	-0.48573	-0.35869

Dipole moment: X = 0.000000 Y = 0.000000 Z = 2.387344
Total Dipole: 2.387344 Debye

Mulliken Population Analysis

AO	ATOM	Occupancy
1	1	0.431950
2	1	0.201625
3	2	1.985248
4	2	0.417366
5	2	0.546263
6	2	0.871639
7	2	0.687943
8	2	1.482456
9	2	0.671328
10	2	1.128361
11	2	0.942247
12	3	0.431950
13	3	0.201625

Atom		Occupancy	Charge
H	1	0.633575	0.366425
O	2	8.732850	-0.732850

```
    H  3     0.633575     0.366425

  Total Charge =  0.000000


  Natural Atomic Orbital Populations

  Nao  Atom   Type   Basis  Occupancy
  ---  ----  ------- -----  ---------

    1  H  1  S        MIN    0.561009
    2  H  1  S        RYD    0.001061
    3  O  2  S        MIN    1.999837
    4  O  2  S        MIN    1.761981
    5  O  2  S        RYD    0.000368
    6  O  2  PX       MIN    1.407314
    7  O  2  PX       RYD    0.000540
    8  O  2  PY       MIN    1.999930
    9  O  2  PY       RYD    0.000070
   10  O  2  PZ       MIN    1.705562
   11  O  2  PZ       RYD    0.000258
   12  H  3  S        MIN    0.561009
   13  H  3  S        RYD    0.001061

  Total MIN occupancy:   9.996642
  Total RYD occupancy:   0.003358
  Total occupancy:      10.000000


  Natural Atomic Populations and Charges

   Atom    Occupancy     Charge
   ----   -----------  -----------

   H  1     0.562070     0.437930
   O  2     8.875860    -0.875860
   H  3     0.562070     0.437930

  Total Charge =  0.000000

Q-minus(NAO) =  -0.8759
Q-plus(NAO)  =   0.4379


  Mulliken Bond Order Matrix

            1         2

   2     0.82751
   3     0.00811   0.82751


   Atomic Valencies

     Atom      Valency
     ----      -------

     H   1     0.835620
     O   2     1.655014
     H   3     0.835620
```

```
 Lowdin Bond Order Matrix

           1         2

  2     0.95872
  3     0.00798   0.95872


  Atomic Valencies

    Atom      Valency
    ----      -------

    H   1     0.966703
    O   2     1.917437
    H   3     0.966703

 Frequencies and reduced mass in atomic units are:

mode     (cm-1)         AU          mass
   1   -0.4148E-12  -0.6511E-32  -0.5256E+25
   2   -0.1059E-12  -0.4242E-33  -0.2914E+28
   3    0.0000E+00   0.0000E+00Infinity
   4    0.4513E-05   0.7708E-18   0.2466E+18
   5    0.1230E-04   0.5729E-17   0.5376E+17
   6    0.2730E-04   0.2819E-16   0.4229E+16
   7     1799.       0.1225        1.684
   8     3812.       0.5500       0.7836
   9     3945.       0.5891        1.073

 Zero-point vibrational energy is    13.662 kcal/mol

 Standard Thermodynamic quantities at   298.15 K  and     1.00 atm

 Translational Enthalpy:        0.889 kcal/mol
 Rotational Enthalpy:           0.889 kcal/mol
 Vibrational Enthalpy:         13.663 kcal/mol

 Translational Entropy:        34.608  cal/mol.K
 Rotational Entropy:           10.476  cal/mol.K
 Vibrational Entropy:           0.003  cal/mol.K

 Total Cpu time:   0 mins.  0.05 secs.
```

```
..Running Spartan Pre-Processor

water


SPARTAN AB INITIO PROGRAM: SGI/R5K        Release 5.0.1
  (Job run on newton)

  WATER

  Calculation started: Tue Oct  6 14:52:51 1998

  Run type: Geometry optimization
            Numerical Frequency
  Model: RHF/6-31G*
  Number of shells:   8
     5 S shells
     2 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  10
  Use of molecular symmetry enabled
  Molecular charge:   0
  Spin multiplicity:  1

                       Cartesian Coordinates (a.u.)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    H  H1          -0.7540552     0.0000000     0.4587188
    O  O1           0.0000000     0.0000000    -0.1146797
    H  H2           0.7540552     0.0000000     0.4587188

  Point Group = CNV Order =  2 Nsymop =  4
  This system has   2 degrees of freedom
   Coordinates read from pre-optimization

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    H  H1           0.0000000    -1.4249584     0.3611889
    O  O1           0.0000000     0.0000000    -0.7223777
    H  H2           0.0000000     1.4249584     0.3611889

  Initial Hessian option
  Hessian will be taken from archive file


Cycle no:   1   Energy =     -76.0107465 rmsG = 0.0000 rmsD = 0.0000

WATER


                       Cartesian Coordinates (a.u.)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    H  H1          -1.4249584     0.0000000     0.8668533
    O  O1           0.0000000     0.0000000    -0.2167133
    H  H2           1.4249584     0.0000000     0.8668533
```

E(HF) = -76.0107465 a.u.

Closed-Shell Molecular Orbital Coefficients

MO:		1	2	3	4	5
Eigenvalues:		-20.55787	-1.34614	-0.71428	-0.57080	-0.49821
		A1	A1	B2	A1	B1
1 H	1 S	0.00032	-0.13303	0.23245	0.14005	0.00000
2 H	1 S	-0.00021	-0.00173	0.10724	0.08277	0.00000
3 O	2 S	0.99462	0.20953	0.00000	0.07309	0.00000
4 O	2 S	0.02117	-0.47576	0.00000	-0.16364	0.00000
5 O	2 PX	0.00000	0.00000	-0.50892	0.00000	0.00000
6 O	2 PY	0.00000	0.00000	0.00000	0.00000	-0.63927
7 O	2 PZ	0.00134	-0.09475	0.00000	0.55778	0.00000
8 O	2 S	0.00415	-0.43531	0.00000	-0.32543	0.00000
9 O	2 PX	0.00000	0.00000	-0.30386	0.00000	0.00000
10 O	2 PY	0.00000	0.00000	0.00000	0.00000	-0.51184
11 O	2 PZ	-0.00046	-0.04981	0.00000	0.40486	0.00000
12 O	2 DXX	-0.00421	-0.02693	0.00000	-0.00079	0.00000
13 O	2 DYY	-0.00394	0.00103	0.00000	-0.01187	0.00000
14 O	2 DZZ	-0.00409	-0.02131	0.00000	0.04630	0.00000
15 O	2 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
16 O	2 DXZ	0.00000	0.00000	-0.05088	0.00000	0.00000
17 O	2 DYZ	0.00000	0.00000	0.00000	0.00000	-0.03417
18 H	3 S	0.00032	-0.13303	-0.23245	0.14005	0.00000
19 H	3 S	-0.00021	-0.00173	-0.10724	0.08277	0.00000

MO:		6	7	8	9	10
Eigenvalues:		0.21302	0.30687	1.03171	1.13339	1.16803
		A1	B2	B2	A1	B1
1 H	1 S	0.05370	-0.04660	0.83946	-0.51764	0.00000
2 H	1 S	1.05155	-1.41335	-0.42069	0.43629	0.00000
3 O	2 S	0.10145	0.00000	0.00000	-0.00237	0.00000
4 O	2 S	-0.05572	0.00000	0.00000	0.89859	0.00000
5 O	2 PX	0.00000	-0.32566	0.08763	0.00000	0.00000
6 O	2 PY	0.00000	0.00000	0.00000	0.00000	-0.96297
7 O	2 PZ	-0.21186	0.00000	0.00000	-0.47326	0.00000
8 O	2 S	-1.43991	0.00000	0.00000	-1.58419	0.00000
9 O	2 PX	0.00000	-0.84079	0.70893	0.00000	0.00000
10 O	2 PY	0.00000	0.00000	0.00000	0.00000	1.03588
11 O	2 PZ	-0.50250	0.00000	0.00000	0.75624	0.00000
12 O	2 DXX	0.05676	0.00000	0.00000	0.18536	0.00000
13 O	2 DYY	0.07281	0.00000	0.00000	0.37596	0.00000
14 O	2 DZZ	0.04478	0.00000	0.00000	0.31717	0.00000
15 O	2 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
16 O	2 DXZ	0.00000	-0.02321	-0.19900	0.00000	0.00000
17 O	2 DYZ	0.00000	0.00000	0.00000	0.00000	0.01404
18 H	3 S	0.05370	0.04660	-0.83946	-0.51764	0.00000
19 H	3 S	1.05155	1.41335	0.42069	0.43629	0.00000

MO:		11	12	13	14	15
Eigenvalues:		1.17847	1.38512	1.43120	2.02056	2.03057
		A1	B2	A1	A1	A2
1 H	1 S	0.69428	-0.10846	-0.30120	0.08059	0.00000

2	H	1	S	-0.36816	0.93477	-0.81232	0.03736	0.00000
3	O	2	S	0.05106	0.00000	-0.08567	0.00748	0.00000
4	O	2	S	0.05270	0.00000	-1.44352	0.07852	0.00000
5	O	2	PX	0.00000	-1.04032	0.00000	0.00000	0.00000
6	O	2	PY	0.00000	0.00000	0.00000	0.00000	0.00000
7	O	2	PZ	-0.73170	0.00000	-0.50119	0.00283	0.00000
8	O	2	S	-0.41152	0.00000	3.63788	-0.23408	0.00000
9	O	2	PX	0.00000	1.54098	0.00000	0.00000	0.00000
10	O	2	PY	0.00000	0.00000	0.00000	0.00000	0.00000
11	O	2	PZ	0.31536	0.00000	1.15829	-0.13057	0.00000
12	O	2	DXX	0.24962	0.00000	-0.64390	-0.56398	0.00000
13	O	2	DYY	-0.08019	0.00000	-0.29309	-0.38526	0.00000
14	O	2	DZZ	0.06366	0.00000	-0.40363	1.01130	0.00000
15	O	2	DXY	0.00000	0.00000	0.00000	0.00000	1.00000
16	O	2	DXZ	0.00000	0.02686	0.00000	0.00000	0.00000
17	O	2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
18	H	3	S	0.69428	0.10846	-0.30120	0.08059	0.00000
19	H	3	S	-0.36816	-0.93477	-0.81232	0.03736	0.00000

MO:				16	17	18	19
Eigenvalues:				2.06723	2.63565	2.96582	3.97772
				B1	A1	B2	A1
1	H	1	S	0.00000	-0.85909	0.97648	0.13683
2	H	1	S	0.00000	-0.14717	-0.02513	-0.55567
3	O	2	S	0.00000	-0.05866	0.00000	-0.46700
4	O	2	S	0.00000	-0.48350	0.00000	0.31990
5	O	2	PX	0.00000	0.00000	-0.00627	0.00000
6	O	2	PY	-0.00833	0.00000	0.00000	0.00000
7	O	2	PZ	0.00000	-0.03597	0.00000	-0.11760
8	O	2	S	0.00000	1.59546	0.00000	3.65012
9	O	2	PX	0.00000	0.00000	0.89909	0.00000
10	O	2	PY	-0.03205	0.00000	0.00000	0.00000
11	O	2	PZ	0.00000	0.74210	0.00000	0.31480
12	O	2	DXX	0.00000	0.77432	0.00000	-1.53488
13	O	2	DYY	0.00000	-1.13135	0.00000	-1.56200
14	O	2	DZZ	0.00000	0.01781	0.00000	-1.54926
15	O	2	DXY	0.00000	0.00000	0.00000	0.00000
16	O	2	DXZ	0.00000	0.00000	1.29548	0.00000
17	O	2	DYZ	0.99932	0.00000	0.00000	0.00000
18	H	3	S	0.00000	-0.85909	-0.97648	0.13683
19	H	3	S	0.00000	-0.14717	0.02513	-0.55567

Estimating Force Constant Matrix by central-differences

System has approximate symmetry Group: CS Order: 1

Problems determining equivalent atoms symmetry turned off

Hessian Estimation Complete

Normal Modes and Vibrational Frequencies (cm-1)

	1826.50			4070.71			4188.95		
	A1			A1			B2		
	X	Y	Z	X	Y	Z	X	Y	Z
1	-0.415	0.000	-0.540	-0.573	0.000	0.391	0.542	0.000	-0.412
2	0.000	0.000	0.271	0.000	0.000	-0.196	-0.272	0.000	0.000

```
  3   0.415  0.000 -0.540    0.573  0.000  0.391    0.542  0.000  0.412


    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  6.08 secs.
  Total Wall time:       0 mins.  6.75 secs.

  Calculation finished: Tue Oct  6 14:52:58 1998

SPARTAN PROPERTIES PACKAGE: SGI/R5K        Release 5.0.1

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -20.55787   -1.34614   -0.71428   -0.57080   -0.49821

                        A1        A1        B1        A1        B2
   1 H   1 S         0.00032   -0.13303    0.23245    0.14005    0.00000
   2 H   1 S        -0.00021   -0.00173    0.10724    0.08277    0.00000
   3 O   2 S         0.99462    0.20953    0.00000    0.07309    0.00000
   4 O   2 S         0.02117   -0.47576    0.00000   -0.16364    0.00000
   5 O   2 PX        0.00000    0.00000   -0.50892    0.00000    0.00000
   6 O   2 PY        0.00000    0.00000    0.00000    0.00000   -0.63927
   7 O   2 PZ        0.00134   -0.09475    0.00000    0.55778    0.00000
   8 O   2 S         0.00415   -0.43531    0.00000   -0.32543    0.00000
   9 O   2 PX        0.00000    0.00000   -0.30386    0.00000    0.00000
  10 O   2 PY        0.00000    0.00000    0.00000    0.00000   -0.51184
  11 O   2 PZ       -0.00046   -0.04981    0.00000    0.40486    0.00000
  12 O   2 DXX      -0.00421   -0.02693    0.00000   -0.00079    0.00000
  13 O   2 DYY      -0.00394    0.00103    0.00000   -0.01187    0.00000
  14 O   2 DZZ      -0.00409   -0.02131    0.00000    0.04630    0.00000
  15 O   2 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  16 O   2 DXZ       0.00000    0.00000   -0.05088    0.00000    0.00000
  17 O   2 DYZ       0.00000    0.00000    0.00000    0.00000   -0.03417
  18 H   3 S         0.00032   -0.13303   -0.23245    0.14005    0.00000
  19 H   3 S        -0.00021   -0.00173   -0.10724    0.08277    0.00000

  MO:                   6         7         8         9        10

  Eigenvalues:      0.21302    0.30687    1.03171    1.13339    1.16803

                        A1        B1        B1        A1        B2
   1 H   1 S         0.05370   -0.04660    0.83946   -0.51764    0.00000
   2 H   1 S         1.05155   -1.41335   -0.42069    0.43629    0.00000
   3 O   2 S         0.10145    0.00000    0.00000   -0.00237    0.00000
   4 O   2 S        -0.05572    0.00000    0.00000    0.89859    0.00000
   5 O   2 PX        0.00000   -0.32566    0.08763    0.00000    0.00000
   6 O   2 PY        0.00000    0.00000    0.00000    0.00000   -0.96297
   7 O   2 PZ       -0.21186    0.00000    0.00000   -0.47326    0.00000
   8 O   2 S        -1.43991    0.00000    0.00000   -1.58419    0.00000
   9 O   2 PX        0.00000   -0.84079    0.70893    0.00000    0.00000
  10 O   2 PY        0.00000    0.00000    0.00000    0.00000    1.03588
  11 O   2 PZ       -0.50250    0.00000    0.00000    0.75624    0.00000
  12 O   2 DXX       0.05676    0.00000    0.00000    0.18536    0.00000
  13 O   2 DYY       0.07281    0.00000    0.00000    0.37596    0.00000
  14 O   2 DZZ       0.04478    0.00000    0.00000    0.31717    0.00000
  15 O   2 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  16 O   2 DXZ       0.00000   -0.02321   -0.19900    0.00000    0.00000
```

```
17 O   2 DYZ       0.00000    0.00000    0.00000    0.00000    0.01404
18 H   3 S         0.05370    0.04660   -0.83946   -0.51764    0.00000
19 H   3 S         1.05155    1.41335    0.42069    0.43629    0.00000

MO:                  11         12         13         14         15

Eigenvalues:       1.17847    1.38512    1.43120    2.02056    2.03057

                     A1         B1         A1         A1         A2
 1 H   1 S         0.69428   -0.10846   -0.30120    0.08059    0.00000
 2 H   1 S        -0.36816    0.93477   -0.81232    0.03736    0.00000
 3 O   2 S         0.05106    0.00000   -0.08567    0.00748    0.00000
 4 O   2 S         0.05270    0.00000   -1.44352    0.07852    0.00000
 5 O   2 PX        0.00000   -1.04032    0.00000    0.00000    0.00000
 6 O   2 PY        0.00000    0.00000    0.00000    0.00000    0.00000
 7 O   2 PZ       -0.73170    0.00000   -0.50119    0.00283    0.00000
 8 O   2 S        -0.41152    0.00000    3.63788   -0.23408    0.00000
 9 O   2 PX        0.00000    1.54098    0.00000    0.00000    0.00000
10 O   2 PY        0.00000    0.00000    0.00000    0.00000    0.00000
11 O   2 PZ        0.31536    0.00000    1.15829   -0.13057    0.00000
12 O   2 DXX       0.24962    0.00000   -0.64390   -0.56398    0.00000
13 O   2 DYY      -0.08019    0.00000   -0.29309   -0.38526    0.00000
14 O   2 DZZ       0.06366    0.00000   -0.40363    1.01130    0.00000
15 O   2 DXY       0.00000    0.00000    0.00000    0.00000    1.00000
16 O   2 DXZ       0.00000    0.02686    0.00000    0.00000    0.00000
17 O   2 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
18 H   3 S         0.69428    0.10846   -0.30120    0.08059    0.00000
19 H   3 S        -0.36816   -0.93477   -0.81232    0.03736    0.00000

MO:                  16         17         18         19

Eigenvalues:       2.06723    2.63565    2.96582    3.97772

                     B2         A1         B1         A1
 1 H   1 S         0.00000   -0.85909    0.97648    0.13683
 2 H   1 S         0.00000   -0.14717   -0.02513   -0.55567
 3 O   2 S         0.00000   -0.05866    0.00000   -0.46700
 4 O   2 S         0.00000   -0.48350    0.00000    0.31990
 5 O   2 PX        0.00000    0.00000   -0.00627    0.00000
 6 O   2 PY       -0.00833    0.00000    0.00000    0.00000
 7 O   2 PZ        0.00000   -0.03597    0.00000   -0.11760
 8 O   2 S         0.00000    1.59546    0.00000    3.65012
 9 O   2 PX        0.00000    0.00000    0.89909    0.00000
10 O   2 PY       -0.03205    0.00000    0.00000    0.00000
11 O   2 PZ        0.00000    0.74210    0.00000    0.31480
12 O   2 DXX       0.00000    0.77432    0.00000   -1.53488
13 O   2 DYY       0.00000   -1.13135    0.00000   -1.56200
14 O   2 DZZ       0.00000    0.01781    0.00000   -1.54926
15 O   2 DXY       0.00000    0.00000    0.00000    0.00000
16 O   2 DXZ       0.00000    0.00000    1.29548    0.00000
17 O   2 DYZ       0.99932    0.00000    0.00000    0.00000
18 H   3 S         0.00000   -0.85909   -0.97648    0.13683
19 H   3 S         0.00000   -0.14717    0.02513   -0.55567

Dipole moment:  X =   0.000000  Y =   0.000000  Z =   2.198922
Total Dipole:   2.198922 Debye

Mulliken Population Analysis

  AO  ATOM      Occupancy
  --  ----      ---------
```

```
   1     1       0.467771
   2     1       0.097850
   3     2       1.995294
   4     2       0.902675
   5     2       0.809455
   6     2       1.145516
   7     2       0.952547
   8     2       0.914121
   9     2       0.521210
  10     2       0.852149
  11     2       0.692808
  12     2       0.037782
  13     2       0.003057
  14     2       0.017877
  15     2       0.000000
  16     2       0.021933
  17     2       0.002335
  18     3       0.467771
  19     3       0.097850

   Atom    Occupancy      Charge
   ----   -----------  -----------

   H  1     0.565621     0.434379
   O  2     8.868758    -0.868758
   H  3     0.565621     0.434379

 Total Charge =  0.000000


 Natural Atomic Orbital Populations

 Nao  Atom   Type    Basis  Occupancy
 ---  ----  ------- -----  ---------

   1  H  1  S        MIN    0.521916
   2  H  1  S        RYD    0.000702
   3  O  2  S        MIN    1.999927
   4  O  2  S        MIN    1.747522
   5  O  2  S        RYD    0.001244
   6  O  2  S        RYD    0.000000
   7  O  2  PX       MIN    1.462179
   8  O  2  PX       RYD    0.001810
   9  O  2  PY       MIN    1.997090
  10  O  2  PY       RYD    0.000575
  11  O  2  PZ       MIN    1.732922
  12  O  2  PZ       RYD    0.000246
  13  O  2  DXY      RYD    0.000000
  14  O  2  DXZ      RYD    0.005024
  15  O  2  DYZ      RYD    0.002335
  16  O  2  DXX-YY   RYD    0.001297
  17  O  2  D3ZZ-RR  RYD    0.002592
  18  H  3  S        MIN    0.521916
  19  H  3  S        RYD    0.000702

 Total MIN occupancy:   9.983473
 Total RYD occupancy:   0.016527
 Total occupancy:      10.000000
```

Natural Atomic Populations and Charges

Atom	Occupancy	Charge
H 1	0.522618	0.477382
O 2	8.954764	-0.954764
H 3	0.522618	0.477382

Total Charge = 0.000000

Q-minus(NAO) = -0.9548
Q-plus(NAO) = 0.4774

Mulliken Bond Order Matrix

	1	2
2	0.78527	
3	-0.00410	0.78527

Atomic Valencies

Atom	Valency
H 1	0.781169
O 2	1.570532
H 3	0.781169

Lowdin Bond Order Matrix

	1	2
2	0.87821	
3	0.00521	0.87821

Atomic Valencies

Atom	Valency
H 1	0.883420
O 2	1.756430
H 3	0.883420

Frequencies and reduced mass in atomic units are:

mode	(cm-1)	AU	mass
1	-0.2081E-04	-0.1639E-16	-0.1701E+17
2	-0.1454E-04	-0.8001E-17	-0.3570E+17
3	-0.2632E-13	-0.2621E-34	0.1086E+30
4	0.4033E-12	0.6156E-32	-0.1010E+28
5	0.2708E-04	0.2776E-16	0.8081E+16
6	0.4177E-04	0.6602E-16	0.3425E+16
7	1826.	0.1262	1.802
8	4071.	0.6271	0.8326
9	4189.	0.6640	1.058

```
 Zero-point vibrational energy is    14.419 kcal/mol

 Standard Thermodynamic quantities at   298.15 K  and     1.00 atm

 Translational Enthalpy:        0.889 kcal/mol
 Rotational Enthalpy:           0.889 kcal/mol
 Vibrational Enthalpy:         14.420 kcal/mol

 Translational Entropy:        34.608  cal/mol.K
 Rotational Entropy:           10.376  cal/mol.K
 Vibrational Entropy:           0.003  cal/mol.K

 Total Cpu time:   0 mins.  0.08 secs.
```

```
..Running Spartan Pre-Processor

water


SPARTAN AB INITIO PROGRAM: SGI/R5K        Release 5.0.1
  (Job run on newton)

  WATER

  Calculation started: Fri Oct  2 15:13:30 1998

  Run type: Geometry optimization
            Numerical Frequency
  Model: RHF/6-311G**
  Number of shells:  13
     7 S shells
     2 P shells
     3 SP shells
     1 5D shells
  Number of basis functions:  30
  Number of electrons:  10
  Use of molecular symmetry enabled
  Molecular charge:   0
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    H  H1          -0.7465799     0.0000000     0.4792601
    O  O1           0.0000000     0.0000000    -0.1198150
    H  H2           0.7465799     0.0000000     0.4792601

  Point Group = CNV Order =  2 Nsymop =  4
  This system has   2 degrees of freedom
   Coordinates read from pre-optimization

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    H  H1           0.0000000    -0.7465799     0.1996917
    O  O1           0.0000000     0.0000000    -0.3993834
    H  H2           0.0000000     0.7465799     0.1996917

  Initial Hessian option
  Hessian will be taken from archive file


Cycle no:   1   Energy =     -76.0463003 rmsG = 0.0122 rmsD = 0.0097

Cycle no:   2   Energy =     -76.0469967 rmsG = 0.0027 rmsD = 0.0020

Cycle no:   3   Energy =     -76.0470119 rmsG = 0.0003 rmsD = 0.0002

Cycle no:   4   Energy =     -76.0470120 rmsG = 0.0001 rmsD = 0.0000

WATER
```

Cartesian Coordinates (Angstroms)

Atom	Label	X	Y	Z
H	H1	-0.7488844	0.0000000	0.4558562
O	O1	0.0000000	0.0000000	-0.1139640
H	H2	0.7488844	0.0000000	0.4558562

E(HF) = -76.0470120 a.u.

Closed-Shell Molecular Orbital Coefficients

MO:	1	2	3	4	5
Eigenvalues:	-20.54134	-1.34911	-0.71720	-0.57284	-0.50066
	A1	A1	B2	A1	B1
1 H 1 S	-0.00021	0.09655	0.15126	-0.08746	0.00000
2 H 1 S	-0.00008	0.08131	0.21226	-0.14600	0.00000
3 H 1 S	-0.00010	-0.00267	0.05449	-0.02727	0.00000
4 H 1 PX	-0.00007	0.02386	0.01871	-0.02972	0.00000
5 H 1 PY	0.00000	0.00000	0.00000	0.00000	0.03153
6 H 1 PZ	0.00001	-0.01441	-0.02567	-0.00957	0.00000
7 O 2 S	-0.55143	-0.11336	0.00000	-0.03814	0.00000
8 O 2 S	-0.47168	-0.18936	0.00000	-0.06486	0.00000
9 O 2 PX	0.00000	0.00000	-0.22737	0.00000	0.00000
10 O 2 PY	0.00000	0.00000	0.00000	0.00000	0.29170
11 O 2 PZ	-0.00179	0.03802	0.00000	-0.25569	0.00000
12 O 2 S	-0.00557	0.53789	0.00000	0.19645	0.00000
13 O 2 PX	0.00000	0.00000	-0.34886	0.00000	0.00000
14 O 2 PY	0.00000	0.00000	0.00000	0.00000	0.43668
15 O 2 PZ	0.00062	0.06314	0.00000	-0.37819	0.00000
16 O 2 S	0.00047	0.37192	0.00000	0.33482	0.00000
17 O 2 PX	0.00000	0.00000	-0.21179	0.00000	0.00000
18 O 2 PY	0.00000	0.00000	0.00000	0.00000	0.46588
19 O 2 PZ	-0.00009	0.02078	0.00000	-0.34001	0.00000
20 O 2 DZ**2	0.00002	0.00276	0.00000	-0.01698	0.00000
21 O 2 DYY-ZZ	0.00012	0.00804	0.00000	-0.00506	0.00000
22 O 2 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
23 O 2 DXZ	0.00000	0.00000	-0.02932	0.00000	0.00000
24 O 2 DYZ	0.00000	0.00000	0.00000	0.00000	0.01714
25 H 3 S	-0.00021	0.09655	-0.15126	-0.08746	0.00000
26 H 3 S	-0.00008	0.08131	-0.21226	-0.14600	0.00000
27 H 3 S	-0.00010	-0.00267	-0.05449	-0.02727	0.00000
28 H 3 PX	0.00007	-0.02386	0.01871	0.02972	0.00000
29 H 3 PY	0.00000	0.00000	0.00000	0.00000	0.03153
30 H 3 PZ	0.00001	-0.01441	0.02567	-0.00957	0.00000

MO:	6	7	8	9	10
Eigenvalues:	0.15259	0.21857	0.57721	0.62066	0.99746
	A1	B2	B2	A1	A1
1 H 1 S	-0.03414	0.02363	0.07981	0.06267	-0.03375
2 H 1 S	0.06825	-0.13010	1.48636	1.85045	-0.57469
3 H 1 S	-0.84441	1.57992	-0.72184	-0.60061	-0.11534
4 H 1 PX	0.00513	-0.00885	0.02621	0.03687	-0.15196
5 H 1 PY	0.00000	0.00000	0.00000	0.00000	0.00000
6 H 1 PZ	0.00381	0.00818	0.00274	-0.04461	0.09942
7 O 2 S	-0.03350	0.00000	0.00000	0.03360	-0.01291
8 O 2 S	-0.05464	0.00000	0.00000	0.05903	-0.02414

9	O	2	PX	0.00000	0.12024	0.12035	0.00000	0.00000
10	O	2	PY	0.00000	0.00000	0.00000	0.00000	0.00000
11	O	2	PZ	0.07159	0.00000	0.00000	-0.09602	-0.23504
12	O	2	S	0.10270	0.00000	0.00000	-0.13501	0.04648
13	O	2	PX	0.00000	0.12748	0.18575	0.00000	0.00000
14	O	2	PY	0.00000	0.00000	0.00000	0.00000	0.00000
15	O	2	PZ	0.11396	0.00000	0.00000	-0.18556	-0.73593
16	O	2	S	0.85278	0.00000	0.00000	-1.48816	0.95078
17	O	2	PX	0.00000	0.49548	1.17086	0.00000	0.00000
18	O	2	PY	0.00000	0.00000	0.00000	0.00000	0.00000
19	O	2	PZ	0.19995	0.00000	0.00000	-1.08819	1.56760
20	O	2	DZ**2	0.00456	0.00000	0.00000	-0.01127	-0.00458
21	O	2	DYY-ZZ	0.00367	0.00000	0.00000	0.00813	0.01773
22	O	2	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
23	O	2	DXZ	0.00000	0.00554	-0.01302	0.00000	0.00000
24	O	2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
25	H	3	S	-0.03414	-0.02363	-0.07981	0.06267	-0.03375
26	H	3	S	0.06825	0.13010	-1.48636	1.85045	-0.57469
27	H	3	S	-0.84441	-1.57992	0.72184	-0.60061	-0.11534
28	H	3	PX	-0.00513	-0.00885	0.02621	-0.03687	0.15196
29	H	3	PY	0.00000	0.00000	0.00000	0.00000	0.00000
30	H	3	PZ	0.00381	-0.00818	-0.00274	-0.04461	0.09942

MO:		11	12	13	14	15
Eigenvalues:		1.00311	1.11139	1.31048	1.49825	1.51587
		B1	B2	A1	A1	A2
1	H	1	S	0.00000	0.01962	-0.00884	-0.08423	0.00000
2	H	1	S	0.00000	0.34721	0.88699	1.20378	0.00000
3	H	1	S	0.00000	0.80104	0.35673	-0.02918	0.00000
4	H	1	PX	0.00000	0.17441	0.18385	0.59805	0.00000
5	H	1	PY	0.02768	0.00000	0.00000	0.00000	0.68970
6	H	1	PZ	0.00000	-0.14572	-0.36900	0.42794	0.00000
7	O	2	S	0.00000	0.00000	-0.09974	-0.03344	0.00000
8	O	2	S	0.00000	0.00000	-0.20421	-0.06934	0.00000
9	O	2	PX	0.00000	-0.24104	0.00000	0.00000	0.00000
10	O	2	PY	0.23940	0.00000	0.00000	0.00000	0.00000
11	O	2	PZ	0.00000	0.00000	0.02803	-0.01484	0.00000
12	O	2	S	0.00000	0.00000	1.48630	0.58510	0.00000
13	O	2	PX	0.00000	-0.70501	0.00000	0.00000	0.00000
14	O	2	PY	0.83601	0.00000	0.00000	0.00000	0.00000
15	O	2	PZ	0.00000	0.00000	-0.17800	-0.12055	0.00000
16	O	2	S	0.00000	0.00000	-3.19000	-2.05767	0.00000
17	O	2	PX	0.00000	1.80252	0.00000	0.00000	0.00000
18	O	2	PY	-1.15631	0.00000	0.00000	0.00000	0.00000
19	O	2	PZ	0.00000	0.00000	-0.58767	-1.24349	0.00000
20	O	2	DZ**2	0.00000	0.00000	-0.02813	0.11649	0.00000
21	O	2	DYY-ZZ	0.00000	0.00000	-0.02491	-0.05730	0.00000
22	O	2	DXY	0.00000	0.00000	0.00000	0.00000	-0.12197
23	O	2	DXZ	0.00000	0.03183	0.00000	0.00000	0.00000
24	O	2	DYZ	0.00840	0.00000	0.00000	0.00000	0.00000
25	H	3	S	0.00000	-0.01962	-0.00884	-0.08423	0.00000
26	H	3	S	0.00000	-0.34721	0.88699	1.20378	0.00000
27	H	3	S	0.00000	-0.80104	0.35673	-0.02918	0.00000
28	H	3	PX	0.00000	0.17441	-0.18385	-0.59805	0.00000
29	H	3	PY	0.02768	0.00000	0.00000	0.00000	-0.68970
30	H	3	PZ	0.00000	0.14572	-0.36900	0.42794	0.00000

MO:	16	17	18	19	20

Eigenvalues:			1.72689	1.93034	2.27741	2.39787	2.61014
			B1	B2	B2	A1	A1
1	H	1 S	0.00000	-0.19084	-0.71308	0.94219	0.43205
2	H	1 S	0.00000	0.78704	0.74227	-1.34110	-1.90376
3	H	1 S	0.00000	-0.16046	-0.54207	0.43142	0.21691
4	H	1 PX	0.00000	-0.48085	-0.24935	0.17382	-0.96203
5	H	1 PY	0.77200	0.00000	0.00000	0.00000	0.00000
6	H	1 PZ	0.00000	-0.65135	0.46729	-0.03340	0.67877
7	O	2 S	0.00000	0.00000	0.00000	0.02416	-0.06006
8	O	2 S	0.00000	0.00000	0.00000	0.04213	-0.14041
9	O	2 PX	0.00000	-0.01516	-0.17653	0.00000	0.00000
10	O	2 PY	-0.05289	0.00000	0.00000	0.00000	0.00000
11	O	2 PZ	0.00000	0.00000	0.00000	-0.16064	0.03958
12	O	2 S	0.00000	0.00000	0.00000	-0.14379	1.00798
13	O	2 PX	0.00000	-0.02756	-0.46807	0.00000	0.00000
14	O	2 PY	-0.07510	0.00000	0.00000	0.00000	0.00000
15	O	2 PZ	0.00000	0.00000	0.00000	-0.15953	0.72070
16	O	2 S	0.00000	0.00000	0.00000	0.41722	1.83751
17	O	2 PX	0.00000	0.94915	0.02699	0.00000	0.00000
18	O	2 PY	-0.55157	0.00000	0.00000	0.00000	0.00000
19	O	2 PZ	0.00000	0.00000	0.00000	0.32938	0.73342
20	O	2 DZ**2	0.00000	0.00000	0.00000	0.07643	-0.04727
21	O	2 DYY-ZZ	0.00000	0.00000	0.00000	0.29305	-0.03211
22	O	2 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
23	O	2 DXZ	0.00000	0.07911	0.25255	0.00000	0.00000
24	O	2 DYZ	0.14548	0.00000	0.00000	0.00000	0.00000
25	H	3 S	0.00000	0.19084	0.71308	0.94219	0.43205
26	H	3 S	0.00000	-0.78704	-0.74227	-1.34110	-1.90376
27	H	3 S	0.00000	0.16046	0.54207	0.43142	0.21691
28	H	3 PX	0.00000	-0.48085	-0.24935	-0.17382	0.96203
29	H	3 PY	0.77200	0.00000	0.00000	0.00000	0.00000
30	H	3 PZ	0.00000	0.65135	-0.46729	-0.03340	0.67877

MO:			21	22	23	24	25
Eigenvalues:			2.76847	3.50524	3.57207	3.73798	4.03524
			B2	B1	A2	A1	A1
1	H	1 S	-0.72908	0.00000	0.00000	0.02703	0.35215
2	H	1 S	2.13086	0.00000	0.00000	0.57242	1.03741
3	H	1 S	-0.50213	0.00000	0.00000	-0.02841	0.05949
4	H	1 PX	0.95005	0.00000	0.00000	0.42416	0.56007
5	H	1 PY	0.00000	0.36679	0.35115	0.00000	0.00000
6	H	1 PZ	-0.68780	0.00000	0.00000	0.23271	-0.48256
7	O	2 S	0.00000	0.00000	0.00000	0.00262	0.02461
8	O	2 S	0.00000	0.00000	0.00000	0.00534	0.04966
9	O	2 PX	0.01507	0.00000	0.00000	0.00000	0.00000
10	O	2 PY	0.00000	-0.02383	0.00000	0.00000	0.00000
11	O	2 PZ	0.00000	0.00000	0.00000	-0.05905	-0.31724
12	O	2 S	0.00000	0.00000	0.00000	0.02934	-0.18769
13	O	2 PX	0.97006	0.00000	0.00000	0.00000	0.00000
14	O	2 PY	0.00000	0.00943	0.00000	0.00000	0.00000
15	O	2 PZ	0.00000	0.00000	0.00000	-0.05054	-0.13202
16	O	2 S	0.00000	0.00000	0.00000	-0.86149	-2.00064
17	O	2 PX	0.73233	0.00000	0.00000	0.00000	0.00000
18	O	2 PY	0.00000	-0.27519	0.00000	0.00000	0.00000
19	O	2 PZ	0.00000	0.00000	0.00000	-0.67660	-0.89584
20	O	2 DZ**2	0.00000	0.00000	0.00000	-1.08345	-0.04810
21	O	2 DYY-ZZ	0.00000	0.00000	0.00000	0.07943	-1.12457
22	O	2 DXY	0.00000	0.00000	1.06005	0.00000	0.00000

23	O	2	DXZ	0.23826	0.00000	0.00000	0.00000	0.00000
24	O	2	DYZ	0.00000	-1.03732	0.00000	0.00000	0.00000
25	H	3	S	0.72908	0.00000	0.00000	0.02703	0.35215
26	H	3	S	-2.13086	0.00000	0.00000	0.57242	1.03741
27	H	3	S	0.50213	0.00000	0.00000	-0.02841	0.05949
28	H	3	PX	0.95005	0.00000	0.00000	-0.42416	-0.56007
29	H	3	PY	0.00000	0.36679	-0.35115	0.00000	0.00000
30	H	3	PZ	0.68780	0.00000	0.00000	0.23271	-0.48256

MO:	26	27	28	29	30
Eigenvalues:	4.28219	5.33047	5.76188	6.25786	51.57497
	B2	B1	A1	B2	A1
1 H 1 S	0.44139	0.00000	0.30691	0.39797	-0.00874
2 H 1 S	0.48389	0.00000	0.52186	0.51199	-0.07770
3 H 1 S	0.24461	0.00000	0.01487	-0.14556	0.03113
4 H 1 PX	0.46733	0.00000	0.48401	0.54694	-0.06568
5 H 1 PY	0.00000	0.06593	0.00000	0.00000	0.00000
6 H 1 PZ	-0.33993	0.00000	-0.26707	-0.47649	0.04814
7 O 2 S	0.00000	0.00000	0.02408	0.00000	2.24732
8 O 2 S	0.00000	0.00000	0.04560	0.00000	-2.33737
9 O 2 PX	0.46759	0.00000	0.00000	-1.25460	0.00000
10 O 2 PY	0.00000	1.27076	0.00000	0.00000	0.00000
11 O 2 PZ	0.00000	0.00000	1.25925	0.00000	-0.01934
12 O 2 S	0.00000	0.00000	-0.26302	0.00000	0.27404
13 O 2 PX	-0.02805	0.00000	0.00000	2.05641	0.00000
14 O 2 PY	0.00000	-1.37564	0.00000	0.00000	0.00000
15 O 2 PZ	0.00000	0.00000	-1.73369	0.00000	0.07717
16 O 2 S	0.00000	0.00000	-1.05978	0.00000	-0.05650
17 O 2 PX	0.92187	0.00000	0.00000	-0.13090	0.00000
18 O 2 PY	0.00000	0.47599	0.00000	0.00000	0.00000
19 O 2 PZ	0.00000	0.00000	0.07814	0.00000	0.01573
20 O 2 DZ**2	0.00000	0.00000	-0.09760	0.00000	0.00337
21 O 2 DYY-ZZ	0.00000	0.00000	-0.37511	0.00000	0.02816
22 O 2 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
23 O 2 DXZ	1.14895	0.00000	0.00000	0.67839	0.00000
24 O 2 DYZ	0.00000	-0.03333	0.00000	0.00000	0.00000
25 H 3 S	-0.44139	0.00000	0.30691	-0.39797	-0.00874
26 H 3 S	-0.48389	0.00000	0.52186	-0.51199	-0.07770
27 H 3 S	-0.24461	0.00000	0.01487	0.14556	0.03113
28 H 3 PX	0.46733	0.00000	-0.48401	0.54694	0.06568
29 H 3 PY	0.00000	0.06593	0.00000	0.00000	0.00000
30 H 3 PZ	0.33993	0.00000	-0.26707	0.47649	0.04814

Estimating Force Constant Matrix by central-differences

System has approximate symmetry Group: CS Order: 1

Problems determining equivalent atoms symmetry turned off

Hessian Estimation Complete

Normal Modes and Vibrational Frequencies (cm-1)

	1751.19			4141.46			4236.69		
	A1			A1			B2		
	X	Y	Z	X	Y	Z	X	Y	Z
1	-0.415	0.000	-0.540	0.572	0.000	-0.391	0.542	0.000	-0.412

```
  2   0.000  0.000  0.271    0.000  0.000  0.196   -0.272  0.000  0.000
  3   0.415  0.000 -0.540   -0.572  0.000 -0.391    0.542  0.000  0.412



    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins. 18.87 secs.
  Total Wall time:       0 mins. 20.31 secs.

  Calculation finished: Fri Oct  2 15:13:50 1998

SPARTAN PROPERTIES PACKAGE: SGI/R5K        Release 5.0.1

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -20.54134  -1.34911  -0.71720  -0.57284  -0.50066

                       A1        A1        B1        A1        B2
   1 H   1 S        -0.00021   0.09655   0.15126  -0.08746   0.00000
   2 H   1 S        -0.00008   0.08131   0.21226  -0.14600   0.00000
   3 H   1 S        -0.00010  -0.00267   0.05449  -0.02727   0.00000
   4 H   1 PX       -0.00007   0.02386   0.01871  -0.02972   0.00000
   5 H   1 PY        0.00000   0.00000   0.00000   0.00000   0.03153
   6 H   1 PZ        0.00001  -0.01441  -0.02567  -0.00957   0.00000
   7 O   2 S        -0.55143  -0.11336   0.00000  -0.03814   0.00000
   8 O   2 S        -0.47168  -0.18936   0.00000  -0.06486   0.00000
   9 O   2 PX        0.00000   0.00000  -0.22737   0.00000   0.00000
  10 O   2 PY        0.00000   0.00000   0.00000   0.00000   0.29170
  11 O   2 PZ       -0.00179   0.03802   0.00000  -0.25569   0.00000
  12 O   2 S        -0.00557   0.53789   0.00000   0.19645   0.00000
  13 O   2 PX        0.00000   0.00000  -0.34886   0.00000   0.00000
  14 O   2 PY        0.00000   0.00000   0.00000   0.00000   0.43668
  15 O   2 PZ        0.00062   0.06314   0.00000  -0.37819   0.00000
  16 O   2 S         0.00047   0.37192   0.00000   0.33482   0.00000
  17 O   2 PX        0.00000   0.00000  -0.21179   0.00000   0.00000
  18 O   2 PY        0.00000   0.00000   0.00000   0.00000   0.46588
  19 O   2 PZ       -0.00009   0.02078   0.00000  -0.34001   0.00000
  20 O   2 DZ**2     0.00002   0.00276   0.00000  -0.01698   0.00000
  21 O   2 DYY-ZZ    0.00012   0.00804   0.00000  -0.00506   0.00000
  22 O   2 DXY       0.00000   0.00000   0.00000   0.00000   0.00000
  23 O   2 DXZ       0.00000   0.00000  -0.02932   0.00000   0.00000
  24 O   2 DYZ       0.00000   0.00000   0.00000   0.00000   0.01714
  25 H   3 S        -0.00021   0.09655  -0.15126  -0.08746   0.00000
  26 H   3 S        -0.00008   0.08131  -0.21226  -0.14600   0.00000
  27 H   3 S        -0.00010  -0.00267  -0.05449  -0.02727   0.00000
  28 H   3 PX        0.00007  -0.02386   0.01871   0.02972   0.00000
  29 H   3 PY        0.00000   0.00000   0.00000   0.00000   0.03153
  30 H   3 PZ        0.00001  -0.01441   0.02567  -0.00957   0.00000

  MO:                   6         7         8         9        10

  Eigenvalues:      0.15259   0.21857   0.57721   0.62066   0.99746

                       A1        B1        B1        A1        A1
   1 H   1 S        -0.03414   0.02363   0.07981   0.06267  -0.03375
   2 H   1 S         0.06825  -0.13010   1.48636   1.85045  -0.57469
   3 H   1 S        -0.84441   1.57992  -0.72184  -0.60061  -0.11534
   4 H   1 PX        0.00513  -0.00885   0.02621   0.03687  -0.15196
```

5	H	1	PY	0.00000	0.00000	0.00000	0.00000	0.00000
6	H	1	PZ	0.00381	0.00818	0.00274	-0.04461	0.09942
7	O	2	S	-0.03350	0.00000	0.00000	0.03360	-0.01291
8	O	2	S	-0.05464	0.00000	0.00000	0.05903	-0.02414
9	O	2	PX	0.00000	0.12024	0.12035	0.00000	0.00000
10	O	2	PY	0.00000	0.00000	0.00000	0.00000	0.00000
11	O	2	PZ	0.07159	0.00000	0.00000	-0.09602	-0.23504
12	O	2	S	0.10270	0.00000	0.00000	-0.13501	0.04648
13	O	2	PX	0.00000	0.12748	0.18575	0.00000	0.00000
14	O	2	PY	0.00000	0.00000	0.00000	0.00000	0.00000
15	O	2	PZ	0.11396	0.00000	0.00000	-0.18556	-0.73593
16	O	2	S	0.85278	0.00000	0.00000	-1.48816	0.95078
17	O	2	PX	0.00000	0.49548	1.17086	0.00000	0.00000
18	O	2	PY	0.00000	0.00000	0.00000	0.00000	0.00000
19	O	2	PZ	0.19995	0.00000	0.00000	-1.08819	1.56760
20	O	2	DZ**2	0.00456	0.00000	0.00000	-0.01127	-0.00458
21	O	2	DYY-ZZ	0.00367	0.00000	0.00000	0.00813	0.01773
22	O	2	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
23	O	2	DXZ	0.00000	0.00554	-0.01302	0.00000	0.00000
24	O	2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
25	H	3	S	-0.03414	-0.02363	-0.07981	0.06267	-0.03375
26	H	3	S	0.06825	0.13010	-1.48636	1.85045	-0.57469
27	H	3	S	-0.84441	-1.57992	0.72184	-0.60061	-0.11534
28	H	3	PX	-0.00513	-0.00885	0.02621	-0.03687	0.15196
29	H	3	PY	0.00000	0.00000	0.00000	0.00000	0.00000
30	H	3	PZ	0.00381	-0.00818	-0.00274	-0.04461	0.09942

MO:				11	12	13	14	15
Eigenvalues:				1.00311	1.11139	1.31048	1.49825	1.51587
				B2	B1	A1	A1	A2
1	H	1	S	0.00000	0.01962	-0.00884	-0.08423	0.00000
2	H	1	S	0.00000	0.34721	0.88699	1.20378	0.00000
3	H	1	S	0.00000	0.80104	0.35673	-0.02918	0.00000
4	H	1	PX	0.00000	0.17441	0.18385	0.59805	0.00000
5	H	1	PY	0.02768	0.00000	0.00000	0.00000	0.68970
6	H	1	PZ	0.00000	-0.14572	-0.36900	0.42794	0.00000
7	O	2	S	0.00000	0.00000	-0.09974	-0.03344	0.00000
8	O	2	S	0.00000	0.00000	-0.20421	-0.06934	0.00000
9	O	2	PX	0.00000	-0.24104	0.00000	0.00000	0.00000
10	O	2	PY	0.23940	0.00000	0.00000	0.00000	0.00000
11	O	2	PZ	0.00000	0.00000	0.02803	-0.01484	0.00000
12	O	2	S	0.00000	0.00000	1.48630	0.58510	0.00000
13	O	2	PX	0.00000	-0.70501	0.00000	0.00000	0.00000
14	O	2	PY	0.83601	0.00000	0.00000	0.00000	0.00000
15	O	2	PZ	0.00000	0.00000	-0.17800	-0.12055	0.00000
16	O	2	S	0.00000	0.00000	-3.19000	-2.05767	0.00000
17	O	2	PX	0.00000	1.80252	0.00000	0.00000	0.00000
18	O	2	PY	-1.15631	0.00000	0.00000	0.00000	0.00000
19	O	2	PZ	0.00000	0.00000	-0.58767	-1.24349	0.00000
20	O	2	DZ**2	0.00000	0.00000	-0.02813	0.11649	0.00000
21	O	2	DYY-ZZ	0.00000	0.00000	-0.02491	-0.05730	0.00000
22	O	2	DXY	0.00000	0.00000	0.00000	0.00000	-0.12197
23	O	2	DXZ	0.00000	0.03183	0.00000	0.00000	0.00000
24	O	2	DYZ	0.00840	0.00000	0.00000	0.00000	0.00000
25	H	3	S	0.00000	-0.01962	-0.00884	-0.08423	0.00000
26	H	3	S	0.00000	-0.34721	0.88699	1.20378	0.00000
27	H	3	S	0.00000	-0.80104	0.35673	-0.02918	0.00000
28	H	3	PX	0.00000	0.17441	-0.18385	-0.59805	0.00000
29	H	3	PY	0.02768	0.00000	0.00000	0.00000	-0.68970

30	H	3	PZ	0.00000	0.14572	-0.36900	0.42794	0.00000

MO:				16	17	18	19	20
Eigenvalues:				1.72689	1.93034	2.27741	2.39787	2.61014
				B2	B1	B1	A1	A1
1	H	1	S	0.00000	-0.19084	-0.71308	0.94219	0.43205
2	H	1	S	0.00000	0.78704	0.74227	-1.34110	-1.90376
3	H	1	S	0.00000	-0.16046	-0.54207	0.43142	0.21691
4	H	1	PX	0.00000	-0.48085	-0.24935	0.17382	-0.96203
5	H	1	PY	0.77200	0.00000	0.00000	0.00000	0.00000
6	H	1	PZ	0.00000	-0.65135	0.46729	-0.03340	0.67877
7	O	2	S	0.00000	0.00000	0.00000	0.02416	-0.06006
8	O	2	S	0.00000	0.00000	0.00000	0.04213	-0.14041
9	O	2	PX	0.00000	-0.01516	-0.17653	0.00000	0.00000
10	O	2	PY	-0.05289	0.00000	0.00000	0.00000	0.00000
11	O	2	PZ	0.00000	0.00000	0.00000	-0.16064	0.03958
12	O	2	S	0.00000	0.00000	0.00000	-0.14379	1.00798
13	O	2	PX	0.00000	-0.02756	-0.46807	0.00000	0.00000
14	O	2	PY	-0.07510	0.00000	0.00000	0.00000	0.00000
15	O	2	PZ	0.00000	0.00000	0.00000	-0.15953	0.72070
16	O	2	S	0.00000	0.00000	0.00000	0.41722	1.83751
17	O	2	PX	0.00000	0.94915	0.02699	0.00000	0.00000
18	O	2	PY	-0.55157	0.00000	0.00000	0.00000	0.00000
19	O	2	PZ	0.00000	0.00000	0.00000	0.32938	0.73342
20	O	2	DZ**2	0.00000	0.00000	0.00000	0.07643	-0.04727
21	O	2	DYY-ZZ	0.00000	0.00000	0.00000	0.29305	-0.03211
22	O	2	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
23	O	2	DXZ	0.00000	0.07911	0.25255	0.00000	0.00000
24	O	2	DYZ	0.14548	0.00000	0.00000	0.00000	0.00000
25	H	3	S	0.00000	0.19084	0.71308	0.94219	0.43205
26	H	3	S	0.00000	-0.78704	-0.74227	-1.34110	-1.90376
27	H	3	S	0.00000	0.16046	0.54207	0.43142	0.21691
28	H	3	PX	0.00000	-0.48085	-0.24935	-0.17382	0.96203
29	H	3	PY	0.77200	0.00000	0.00000	0.00000	0.00000
30	H	3	PZ	0.00000	0.65135	-0.46729	-0.03340	0.67877

MO:				21	22	23	24	25
Eigenvalues:				2.76847	3.50524	3.57207	3.73798	4.03524
				B1	B2	A2	A1	A1
1	H	1	S	-0.72908	0.00000	0.00000	0.02703	0.35215
2	H	1	S	2.13086	0.00000	0.00000	0.57242	1.03741
3	H	1	S	-0.50213	0.00000	0.00000	-0.02841	0.05949
4	H	1	PX	0.95005	0.00000	0.00000	0.42416	0.56007
5	H	1	PY	0.00000	0.36679	0.35115	0.00000	0.00000
6	H	1	PZ	-0.68780	0.00000	0.00000	0.23271	-0.48256
7	O	2	S	0.00000	0.00000	0.00000	0.00262	0.02461
8	O	2	S	0.00000	0.00000	0.00000	0.00534	0.04966
9	O	2	PX	0.01507	0.00000	0.00000	0.00000	0.00000
10	O	2	PY	0.00000	-0.02383	0.00000	0.00000	0.00000
11	O	2	PZ	0.00000	0.00000	0.00000	-0.05905	-0.31724
12	O	2	S	0.00000	0.00000	0.00000	0.02934	-0.18769
13	O	2	PX	0.97006	0.00000	0.00000	0.00000	0.00000
14	O	2	PY	0.00000	0.00943	0.00000	0.00000	0.00000
15	O	2	PZ	0.00000	0.00000	0.00000	-0.05054	-0.13202
16	O	2	S	0.00000	0.00000	0.00000	-0.86149	-2.00064
17	O	2	PX	0.73233	0.00000	0.00000	0.00000	0.00000
18	O	2	PY	0.00000	-0.27519	0.00000	0.00000	0.00000

19	O	2	PZ	0.00000	0.00000	0.00000	-0.67660	-0.89584
20	O	2	DZ**2	0.00000	0.00000	0.00000	-1.08345	-0.04810
21	O	2	DYY-ZZ	0.00000	0.00000	0.00000	0.07943	-1.12457
22	O	2	DXY	0.00000	0.00000	1.06005	0.00000	0.00000
23	O	2	DXZ	0.23826	0.00000	0.00000	0.00000	0.00000
24	O	2	DYZ	0.00000	-1.03732	0.00000	0.00000	0.00000
25	H	3	S	0.72908	0.00000	0.00000	0.02703	0.35215
26	H	3	S	-2.13086	0.00000	0.00000	0.57242	1.03741
27	H	3	S	0.50213	0.00000	0.00000	-0.02841	0.05949
28	H	3	PX	0.95005	0.00000	0.00000	-0.42416	-0.56007
29	H	3	PY	0.00000	0.36679	-0.35115	0.00000	0.00000
30	H	3	PZ	0.68780	0.00000	0.00000	0.23271	-0.48256

MO:	26	27	28	29	30
Eigenvalues:	4.28219	5.33047	5.76188	6.25786	51.57497

				B1	B2	A1	B1	A1
1	H	1	S	0.44139	0.00000	0.30691	0.39797	-0.00874
2	H	1	S	0.48389	0.00000	0.52186	0.51199	-0.07770
3	H	1	S	0.24461	0.00000	0.01487	-0.14556	0.03113
4	H	1	PX	0.46733	0.00000	0.48401	0.54694	-0.06568
5	H	1	PY	0.00000	0.06593	0.00000	0.00000	0.00000
6	H	1	PZ	-0.33993	0.00000	-0.26707	-0.47649	0.04814
7	O	2	S	0.00000	0.00000	0.02408	0.00000	2.24732
8	O	2	S	0.00000	0.00000	0.04560	0.00000	-2.33737
9	O	2	PX	0.46759	0.00000	0.00000	-1.25460	0.00000
10	O	2	PY	0.00000	1.27076	0.00000	0.00000	0.00000
11	O	2	PZ	0.00000	0.00000	1.25925	0.00000	-0.01934
12	O	2	S	0.00000	0.00000	-0.26302	0.00000	0.27404
13	O	2	PX	-0.02805	0.00000	0.00000	2.05641	0.00000
14	O	2	PY	0.00000	-1.37564	0.00000	0.00000	0.00000
15	O	2	PZ	0.00000	0.00000	-1.73369	0.00000	0.07717
16	O	2	S	0.00000	0.00000	-1.05978	0.00000	-0.05650
17	O	2	PX	0.92187	0.00000	0.00000	-0.13090	0.00000
18	O	2	PY	0.00000	0.47599	0.00000	0.00000	0.00000
19	O	2	PZ	0.00000	0.00000	0.07814	0.00000	0.01573
20	O	2	DZ**2	0.00000	0.00000	-0.09760	0.00000	0.00337
21	O	2	DYY-ZZ	0.00000	0.00000	-0.37511	0.00000	0.02816
22	O	2	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
23	O	2	DXZ	1.14895	0.00000	0.00000	0.67839	0.00000
24	O	2	DYZ	0.00000	-0.03333	0.00000	0.00000	0.00000
25	H	3	S	-0.44139	0.00000	0.30691	-0.39797	-0.00874
26	H	3	S	-0.48389	0.00000	0.52186	-0.51199	-0.07770
27	H	3	S	-0.24461	0.00000	0.01487	0.14556	0.03113
28	H	3	PX	0.46733	0.00000	-0.48401	0.54694	0.06568
29	H	3	PY	0.00000	0.06593	0.00000	0.00000	0.00000
30	H	3	PZ	0.33993	0.00000	-0.26707	0.47649	0.04814

Dipole moment: X = 0.000000 Y = 0.000000 Z = 2.137708
Total Dipole: 2.137708 Debye

Mulliken Population Analysis

AO	ATOM	Occupancy
1	1	0.272958
2	1	0.379924
3	1	0.025922
4	1	0.027821

```
    5     1       0.022568
    6     1       0.021655
    7     2       1.083442
    8     2       0.912383
    9     2       0.250684
   10     2       0.382610
   11     2       0.309965
   12     2       0.980505
   13     2       0.597741
   14     2       0.806504
   15     2       0.682185
   16     2       0.793039
   17     2       0.357100
   18     2       0.764768
   19     2       0.564735
   20     2       0.001222
   21     2       0.001366
   22     2       0.000000
   23     2       0.009072
   24     2       0.000983
   25     3       0.272958
   26     3       0.379924
   27     3       0.025922
   28     3       0.027821
   29     3       0.022568
   30     3       0.021655

    Atom    Occupancy      Charge
    ----   -----------  -----------

    H  1     0.750848     0.249152
    O  2     8.498304    -0.498304
    H  3     0.750848     0.249152

 Total Charge =  0.000000


 Natural Atomic Orbital Populations

 Nao  Atom   Type   Basis  Occupancy
 ---  ----  ------- -----  ---------

   1  H  1  S        MIN    0.548952
   2  H  1  S        RYD    0.002077
   3  H  1  S        RYD    0.000078
   4  H  1  PX       RYD    0.000740
   5  H  1  PY       RYD    0.001331
   6  H  1  PZ       RYD    0.000846
   7  O  2  S        MIN    1.999846
   8  O  2  S        MIN    1.729481
   9  O  2  S        RYD    0.000536
  10  O  2  S        RYD    0.000000
  11  O  2  PX       MIN    1.437897
  12  O  2  PX       RYD    0.002175
  13  O  2  PX       RYD    0.000000
  14  O  2  PY       MIN    1.995130
  15  O  2  PY       RYD    0.000919
  16  O  2  PY       RYD    0.000000
  17  O  2  PZ       MIN    1.717558
  18  O  2  PZ       RYD    0.000145
  19  O  2  PZ       RYD    0.000020
```

```
   20  O  2  DXY      RYD    0.000000
   21  O  2  DXZ      RYD    0.004303
   22  O  2  DYZ      RYD    0.001290
   23  O  2  DXX-YY   RYD    0.001092
   24  O  2  D3ZZ-RR  RYD    0.001562
   25  H  3  S        MIN    0.548952
   26  H  3  S        RYD    0.002077
   27  H  3  S        RYD    0.000078
   28  H  3  PX       RYD    0.000740
   29  H  3  PY       RYD    0.001331
   30  H  3  PZ       RYD    0.000846

  Total MIN occupancy:   9.977815
  Total RYD occupancy:   0.022185
  Total occupancy:      10.000000


  Natural Atomic Populations and Charges

   Atom    Occupancy     Charge
   ----   -----------  -----------

   H  1     0.554023     0.445977
   O  2     8.891954    -0.891954
   H  3     0.554023     0.445977

  Total Charge =  0.000000

Q-minus(NAO) =  -0.8920
Q-plus(NAO)  =   0.4460


  Mulliken Bond Order Matrix

            1         2

   2     0.96290
   3     0.00727   0.96290


   Atomic Valencies

     Atom      Valency
     ----      -------

     H   1     0.970169
     O   2     1.925804
     H   3     0.970169

  Lowdin Bond Order Matrix

            1         2

   2     1.19097
   3     0.07100   1.19097


   Atomic Valencies

     Atom      Valency
     ----      -------
```

```
    H   1     1.261973
    O   2     2.381937
    H   3     1.261973

 Frequencies and reduced mass in atomic units are:

mode     (cm-1)         AU          mass
   1   -0.3562E-04  -0.4802E-16  -0.6281E+16
   2   -0.1798E-04  -0.1223E-16  -0.1863E+17
   3   -0.5693E-12  -0.1227E-31  -0.2275E+28
   4    0.0000E+00   0.0000E+00Infinity
   5    0.2959E-13   0.3312E-34  -0.1950E+30
   6    0.4916E-04   0.9147E-16   0.3380E+16
   7     1751.       0.1161        1.897
   8     4141.       0.6491       0.8286
   9     4237.       0.6793        1.058

 Zero-point vibrational energy is    14.481 kcal/mol

 Standard Thermodynamic quantities at   298.15 K  and     1.00 atm

 Translational Enthalpy:        0.889 kcal/mol
 Rotational Enthalpy:           0.889 kcal/mol
 Vibrational Enthalpy:         14.482 kcal/mol

 Translational Entropy:        34.608  cal/mol.K
 Rotational Entropy:           10.336  cal/mol.K
 Vibrational Entropy:           0.004  cal/mol.K

 Total Cpu time:   0 mins.  0.14 secs.
```

```
..Running Spartan Pre-Processor

water


SPARTAN AB INITIO PROGRAM: SGI/R5K        Release 5.0.1
  (Job run on newton)

  WATER

  Calculation started: Fri Oct  2 14:44:32 1998

  Run type: Geometry optimization
            Numerical Frequency
  Model: RMP2(FU)/6-311G**
  Number of shells:  13
     7 S shells
     2 P shells
     3 SP shells
     1 5D shells
  Number of basis functions:  30
  Number of electrons:  10
  Use of molecular symmetry enabled
  Molecular charge:   0
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    H  H1          -0.7465799     0.0000000     0.4792601
    O  O1           0.0000000     0.0000000    -0.1198150
    H  H2           0.7465799     0.0000000     0.4792601

  Point Group = CNV Order =  2 Nsymop =  4
  This system has   2 degrees of freedom
   Coordinates read from pre-optimization

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    H  H1           0.0000000    -0.7465799     0.1996917
    O  O1           0.0000000     0.0000000    -0.3993834
    H  H2           0.0000000     0.7465799     0.1996917

  Initial Hessian option
  Hessian will be taken from archive file

  Full MP2 gradient density matrices computed

Cycle no:   1   Energy =     -76.2828958 rmsG = 0.0000 rmsD = 0.0000

WATER


                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    H  H1          -0.7465799     0.0000000     0.4792601
```

```
  O  O1           0.0000000     0.0000000    -0.1198150
  H  H2           0.7465799     0.0000000     0.4792601

E(HF)  =     -76.0463003 a.u.
E(MP2) =     -76.2828958 a.u.

Closed-Shell Molecular Orbital Coefficients

MO:                   1         2         3         4         5

Eigenvalues:     -20.54599   -1.34301   -0.70261   -0.57593   -0.50052

                       A1        A1        B2        A1        B1
 1 H   1 S         0.00020   0.09400  -0.14839   0.08921   0.00000
 2 H   1 S         0.00011   0.08124  -0.21340   0.15338   0.00000
 3 H   1 S         0.00009  -0.00244  -0.05916   0.02886   0.00000
 4 H   1 PX        0.00008   0.02346  -0.01818   0.03082   0.00000
 5 H   1 PY        0.00000   0.00000   0.00000   0.00000   0.03104
 6 H   1 PZ       -0.00003  -0.01508   0.02672   0.00771   0.00000
 7 O   2 S         0.55145  -0.11340   0.00000   0.03881   0.00000
 8 O   2 S         0.47169  -0.18948   0.00000   0.06596   0.00000
 9 O   2 PX        0.00000   0.00000   0.22684   0.00000   0.00000
10 O   2 PY        0.00000   0.00000   0.00000   0.00000   0.29221
11 O   2 PZ        0.00180   0.03739   0.00000   0.25320   0.00000
12 O   2 S         0.00548   0.53965   0.00000  -0.19940   0.00000
13 O   2 PX        0.00000   0.00000   0.34857   0.00000   0.00000
14 O   2 PY        0.00000   0.00000   0.00000   0.00000   0.43724
15 O   2 PZ       -0.00065   0.06269   0.00000   0.37452   0.00000
16 O   2 S        -0.00047   0.37573   0.00000  -0.34022   0.00000
17 O   2 PX        0.00000   0.00000   0.21818   0.00000   0.00000
18 O   2 PY        0.00000   0.00000   0.00000   0.00000   0.46605
19 O   2 PZ        0.00009   0.02088   0.00000   0.33175   0.00000
20 O   2 DZ**2    -0.00002   0.00327   0.00000   0.01712   0.00000
21 O   2 DYY-ZZ   -0.00014   0.00739   0.00000   0.00483   0.00000
22 O   2 DXY       0.00000   0.00000   0.00000   0.00000   0.00000
23 O   2 DXZ       0.00000   0.00000   0.02907   0.00000   0.00000
24 O   2 DYZ       0.00000   0.00000   0.00000   0.00000   0.01719
25 H   3 S         0.00020   0.09400   0.14839   0.08921   0.00000
26 H   3 S         0.00011   0.08124   0.21340   0.15338   0.00000
27 H   3 S         0.00009  -0.00244   0.05916   0.02886   0.00000
28 H   3 PX       -0.00008  -0.02346  -0.01818  -0.03082   0.00000
29 H   3 PY        0.00000   0.00000   0.00000   0.00000   0.03104
30 H   3 PZ       -0.00003  -0.01508  -0.02672   0.00771   0.00000

MO:                   6         7         8         9        10

Eigenvalues:      0.14979   0.21729   0.56316   0.61934   0.99906

                       A1        B2        B2        A1        A1
 1 H   1 S        -0.03518   0.02677  -0.08420   0.06190  -0.03303
 2 H   1 S         0.07062  -0.12332  -1.43073   1.82022  -0.61264
 3 H   1 S        -0.83785   1.57295   0.75990  -0.62256  -0.09840
 4 H   1 PX        0.00619  -0.00835  -0.02098   0.03177  -0.14895
 5 H   1 PY        0.00000   0.00000   0.00000   0.00000   0.00000
 6 H   1 PZ        0.00291   0.00852  -0.00360  -0.03801   0.11045
 7 O   2 S        -0.03321   0.00000   0.00000   0.03375  -0.01513
 8 O   2 S        -0.05414   0.00000   0.00000   0.05917  -0.02819
 9 O   2 PX        0.00000   0.12342  -0.12106   0.00000   0.00000
10 O   2 PY        0.00000   0.00000   0.00000   0.00000   0.00000
11 O   2 PZ        0.07590   0.00000   0.00000  -0.10398  -0.23289
12 O   2 S         0.10255   0.00000   0.00000  -0.13690   0.06103
```

13	O	2	PX	0.00000	0.13237	-0.18251	0.00000	0.00000
14	O	2	PY	0.00000	0.00000	0.00000	0.00000	0.00000
15	O	2	PZ	0.11897	0.00000	0.00000	-0.19554	-0.73304
16	O	2	S	0.83473	0.00000	0.00000	-1.37814	0.94633
17	O	2	PX	0.00000	0.50248	-1.08125	0.00000	0.00000
18	O	2	PY	0.00000	0.00000	0.00000	0.00000	0.00000
19	O	2	PZ	0.21003	0.00000	0.00000	-1.08157	1.60243
20	O	2	DZ**2	0.00498	0.00000	0.00000	-0.01073	-0.00311
21	O	2	DYY-ZZ	0.00282	0.00000	0.00000	0.00943	0.01568
22	O	2	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
23	O	2	DXZ	0.00000	0.00479	0.01471	0.00000	0.00000
24	O	2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
25	H	3	S	-0.03518	-0.02677	0.08420	0.06190	-0.03303
26	H	3	S	0.07062	0.12332	1.43073	1.82022	-0.61264
27	H	3	S	-0.83785	-1.57295	-0.75990	-0.62256	-0.09840
28	H	3	PX	-0.00619	-0.00835	-0.02098	-0.03177	0.14895
29	H	3	PY	0.00000	0.00000	0.00000	0.00000	0.00000
30	H	3	PZ	0.00291	-0.00852	0.00360	-0.03801	0.11045

MO:				11	12	13	14	15
Eigenvalues:				1.00320	1.11056	1.31556	1.45800	1.52184
				B1	B2	A1	A1	A2
1	H	1	S	0.00000	-0.01418	0.01278	0.08131	0.00000
2	H	1	S	0.00000	-0.33725	-0.88500	-1.16796	0.00000
3	H	1	S	0.00000	-0.78435	-0.33585	0.01804	0.00000
4	H	1	PX	0.00000	-0.16614	-0.14914	-0.60886	0.00000
5	H	1	PY	0.02020	0.00000	0.00000	0.00000	0.69071
6	H	1	PZ	0.00000	0.14814	0.37726	-0.38924	0.00000
7	O	2	S	0.00000	0.00000	0.09928	0.03509	0.00000
8	O	2	S	0.00000	0.00000	0.20427	0.07297	0.00000
9	O	2	PX	0.00000	0.24019	0.00000	0.00000	0.00000
10	O	2	PY	0.23996	0.00000	0.00000	0.00000	0.00000
11	O	2	PZ	0.00000	0.00000	-0.02928	0.01171	0.00000
12	O	2	S	0.00000	0.00000	-1.50196	-0.61744	0.00000
13	O	2	PX	0.00000	0.71715	0.00000	0.00000	0.00000
14	O	2	PY	0.83671	0.00000	0.00000	0.00000	0.00000
15	O	2	PZ	0.00000	0.00000	0.15834	0.10991	0.00000
16	O	2	S	0.00000	0.00000	3.13195	2.04767	0.00000
17	O	2	PX	0.00000	-1.78009	0.00000	0.00000	0.00000
18	O	2	PY	-1.15097	0.00000	0.00000	0.00000	0.00000
19	O	2	PZ	0.00000	0.00000	0.61973	1.24002	0.00000
20	O	2	DZ**2	0.00000	0.00000	0.03367	-0.10962	0.00000
21	O	2	DYY-ZZ	0.00000	0.00000	0.01471	0.05939	0.00000
22	O	2	DXY	0.00000	0.00000	0.00000	0.00000	-0.12479
23	O	2	DXZ	0.00000	-0.03011	0.00000	0.00000	0.00000
24	O	2	DYZ	0.00824	0.00000	0.00000	0.00000	0.00000
25	H	3	S	0.00000	0.01418	0.01278	0.08131	0.00000
26	H	3	S	0.00000	0.33725	-0.88500	-1.16796	0.00000
27	H	3	S	0.00000	0.78435	-0.33585	0.01804	0.00000
28	H	3	PX	0.00000	-0.16614	0.14914	0.60886	0.00000
29	H	3	PY	0.02020	0.00000	0.00000	0.00000	-0.69071
30	H	3	PZ	0.00000	-0.14814	0.37726	-0.38924	0.00000

MO:				16	17	18	19	20
Eigenvalues:				1.70567	1.93682	2.23909	2.39330	2.59470
				B1	B2	B2	A1	A1
1	H	1	S	0.00000	-0.19286	-0.67506	0.88727	0.55707

2	H	1	S	0.00000	0.74058	0.67504	-1.09387	-1.98125
3	H	1	S	0.00000	-0.16485	-0.53530	0.41175	0.26521
4	H	1	PX	0.00000	-0.48481	-0.29292	0.28841	-0.88058
5	H	1	PY	0.76517	0.00000	0.00000	0.00000	0.00000
6	H	1	PZ	0.00000	-0.65192	0.48640	-0.14126	0.68496
7	O	2	S	0.00000	0.00000	0.00000	0.03004	-0.05552
8	O	2	S	0.00000	0.00000	0.00000	0.05617	-0.12967
9	O	2	PX	0.00000	-0.01053	-0.17002	0.00000	0.00000
10	O	2	PY	-0.04918	0.00000	0.00000	0.00000	0.00000
11	O	2	PZ	0.00000	0.00000	0.00000	-0.16744	0.02276
12	O	2	S	0.00000	0.00000	0.00000	-0.24095	0.90481
13	O	2	PX	0.00000	-0.00869	-0.48123	0.00000	0.00000
14	O	2	PY	-0.05278	0.00000	0.00000	0.00000	0.00000
15	O	2	PZ	0.00000	0.00000	0.00000	-0.24415	0.68925
16	O	2	S	0.00000	0.00000	0.00000	0.13888	1.78476
17	O	2	PX	0.00000	0.88269	0.00364	0.00000	0.00000
18	O	2	PY	-0.55397	0.00000	0.00000	0.00000	0.00000
19	O	2	PZ	0.00000	0.00000	0.00000	0.23649	0.75532
20	O	2	DZ**2	0.00000	0.00000	0.00000	0.09033	-0.01256
21	O	2	DYY-ZZ	0.00000	0.00000	0.00000	0.27646	-0.00898
22	O	2	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
23	O	2	DXZ	0.00000	0.07493	0.23405	0.00000	0.00000
24	O	2	DYZ	0.14640	0.00000	0.00000	0.00000	0.00000
25	H	3	S	0.00000	0.19286	0.67506	0.88727	0.55707
26	H	3	S	0.00000	-0.74058	-0.67504	-1.09387	-1.98125
27	H	3	S	0.00000	0.16485	0.53530	0.41175	0.26521
28	H	3	PX	0.00000	-0.48481	-0.29292	-0.28841	0.88058
29	H	3	PY	0.76517	0.00000	0.00000	0.00000	0.00000
30	H	3	PZ	0.00000	0.65192	-0.48640	-0.14126	0.68496

MO:	21	22	23	24	25
Eigenvalues:	2.78656	3.50553	3.54430	3.72231	3.99864
	B2	B1	A2	A1	A1
1 H 1 S	-0.79018	0.00000	0.00000	-0.01712	0.31610
2 H 1 S	2.08233	0.00000	0.00000	-0.39987	1.09398
3 H 1 S	-0.52880	0.00000	0.00000	0.02542	0.04578
4 H 1 PX	0.90048	0.00000	0.00000	-0.34670	0.57430
5 H 1 PY	0.00000	0.36127	0.33765	0.00000	0.00000
6 H 1 PZ	-0.63450	0.00000	0.00000	-0.26543	-0.46534
7 O 2 S	0.00000	0.00000	0.00000	0.00053	0.02218
8 O 2 S	0.00000	0.00000	0.00000	0.00156	0.04406
9 O 2 PX	0.01179	0.00000	0.00000	0.00000	0.00000
10 O 2 PY	0.00000	-0.01983	0.00000	0.00000	0.00000
11 O 2 PZ	0.00000	0.00000	0.00000	0.03202	-0.30870
12 O 2 S	0.00000	0.00000	0.00000	-0.06757	-0.11846
13 O 2 PX	0.88076	0.00000	0.00000	0.00000	0.00000
14 O 2 PY	0.00000	0.01424	0.00000	0.00000	0.00000
15 O 2 PZ	0.00000	0.00000	0.00000	0.01207	-0.12952
16 O 2 S	0.00000	0.00000	0.00000	0.59744	-2.05336
17 O 2 PX	0.65083	0.00000	0.00000	0.00000	0.00000
18 O 2 PY	0.00000	-0.26991	0.00000	0.00000	0.00000
19 O 2 PZ	0.00000	0.00000	0.00000	0.55547	-0.99074
20 O 2 DZ**2	0.00000	0.00000	0.00000	1.06452	-0.19938
21 O 2 DYY-ZZ	0.00000	0.00000	0.00000	-0.21650	-1.09932
22 O 2 DXY	0.00000	0.00000	1.05209	0.00000	0.00000
23 O 2 DXZ	0.23174	0.00000	0.00000	0.00000	0.00000
24 O 2 DYZ	0.00000	-1.03612	0.00000	0.00000	0.00000
25 H 3 S	0.79018	0.00000	0.00000	-0.01712	0.31610
26 H 3 S	-2.08233	0.00000	0.00000	-0.39987	1.09398

```
 27 H   3 S         0.52880    0.00000    0.00000    0.02542    0.04578
 28 H   3 PX        0.90048    0.00000    0.00000    0.34670   -0.57430
 29 H   3 PY        0.00000    0.36127   -0.33765    0.00000    0.00000
 30 H   3 PZ        0.63450    0.00000    0.00000   -0.26543   -0.46534

 MO:                  26         27         28         29         30

 Eigenvalues:      4.27434    5.32594    5.76281    6.17867   51.55007

                      B2         B1         A1         B2         A1
  1 H   1 S         0.40780    0.00000    0.28879    0.34577   -0.00560
  2 H   1 S         0.50130    0.00000    0.49321    0.48971   -0.06533
  3 H   1 S         0.23117    0.00000    0.01365   -0.15210    0.03041
  4 H   1 PX        0.46086    0.00000    0.46235    0.50981   -0.05750
  5 H   1 PY        0.00000    0.05881    0.00000    0.00000    0.00000
  6 H   1 PZ       -0.36941    0.00000   -0.27987   -0.46713    0.04572
  7 O   2 S         0.00000    0.00000    0.02261    0.00000    2.24716
  8 O   2 S         0.00000    0.00000    0.04241    0.00000   -2.33609
  9 O   2 PX        0.45261    0.00000    0.00000   -1.25404    0.00000
 10 O   2 PY        0.00000    1.27047    0.00000    0.00000    0.00000
 11 O   2 PZ        0.00000    0.00000    1.26271    0.00000   -0.01847
 12 O   2 S         0.00000    0.00000   -0.22527    0.00000    0.26644
 13 O   2 PX       -0.03633    0.00000    0.00000    1.98589    0.00000
 14 O   2 PY        0.00000   -1.37394    0.00000    0.00000    0.00000
 15 O   2 PZ        0.00000    0.00000   -1.72501    0.00000    0.07168
 16 O   2 S         0.00000    0.00000   -1.01488    0.00000   -0.07433
 17 O   2 PX        0.91370    0.00000    0.00000   -0.15896    0.00000
 18 O   2 PY        0.00000    0.48123    0.00000    0.00000    0.00000
 19 O   2 PZ        0.00000    0.00000    0.08461    0.00000    0.00932
 20 O   2 DZ**2     0.00000    0.00000   -0.11479    0.00000    0.00419
 21 O   2 DYY-ZZ    0.00000    0.00000   -0.35502    0.00000    0.02419
 22 O   2 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
 23 O   2 DXZ       1.15645    0.00000    0.00000    0.65292    0.00000
 24 O   2 DYZ       0.00000   -0.02862    0.00000    0.00000    0.00000
 25 H   3 S        -0.40780    0.00000    0.28879   -0.34577   -0.00560
 26 H   3 S        -0.50130    0.00000    0.49321   -0.48971   -0.06533
 27 H   3 S        -0.23117    0.00000    0.01365    0.15210    0.03041
 28 H   3 PX        0.46086    0.00000   -0.46235    0.50981    0.05750
 29 H   3 PY        0.00000    0.05881    0.00000    0.00000    0.00000
 30 H   3 PZ        0.36941    0.00000   -0.27987    0.46713    0.04572

Estimating Force Constant Matrix by central-differences

 Full MP2 gradient density matrices computed
 Full MP2 gradient density matrices computed

System has approximate symmetry  Group: CS  Order:   1

Problems determining equivalent atoms symmetry turned off
 Full MP2 gradient density matrices computed
 Full MP2 gradient density matrices computed
 Full MP2 gradient density matrices computed
 Full MP2 gradient density matrices computed

System has approximate symmetry  Group: CNV Order:   2

Problems determining equivalent atoms symmetry turned off
 Full MP2 gradient density matrices computed
 Full MP2 gradient density matrices computed
 Full MP2 gradient density matrices computed
```

Hessian Estimation Complete

Normal Modes and Vibrational Frequencies (cm-1)

	1667.11			3909.99			4017.63		
	A1			A1			B2		
	X	Y	Z	X	Y	Z	X	Y	Z
1	-0.421	0.000	-0.536	0.568	0.000	-0.396	0.532	0.000	-0.426
2	0.000	0.000	0.269	0.000	0.000	0.199	-0.267	0.000	0.000
3	0.421	0.000	-0.536	-0.568	0.000	-0.396	0.532	0.000	0.426

** Archive file written to unit 12 **

Total Cpu time: 0 mins. 33.17 secs.
Total Wall time: 0 mins. 34.70 secs.

Calculation finished: Fri Oct 2 14:45:07 1998

SPARTAN PROPERTIES PACKAGE: SGI/R5K Release 5.0.1

Closed-Shell Molecular Orbital Coefficients

MO:		1	2	3	4	5
Eigenvalues:		-20.54599	-1.34301	-0.70261	-0.57593	-0.50052
		A1	A1	B1	A1	B2
1	H 1 S	0.00020	0.09400	-0.14839	0.08921	0.00000
2	H 1 S	0.00011	0.08124	-0.21340	0.15338	0.00000
3	H 1 S	0.00009	-0.00244	-0.05916	0.02886	0.00000
4	H 1 PX	0.00008	0.02346	-0.01818	0.03082	0.00000
5	H 1 PY	0.00000	0.00000	0.00000	0.00000	0.03104
6	H 1 PZ	-0.00003	-0.01508	0.02672	0.00771	0.00000
7	O 2 S	0.55145	-0.11340	0.00000	0.03881	0.00000
8	O 2 S	0.47169	-0.18948	0.00000	0.06596	0.00000
9	O 2 PX	0.00000	0.00000	0.22684	0.00000	0.00000
10	O 2 PY	0.00000	0.00000	0.00000	0.00000	0.29221
11	O 2 PZ	0.00180	0.03739	0.00000	0.25320	0.00000
12	O 2 S	0.00548	0.53965	0.00000	-0.19940	0.00000
13	O 2 PX	0.00000	0.00000	0.34857	0.00000	0.00000
14	O 2 PY	0.00000	0.00000	0.00000	0.00000	0.43724
15	O 2 PZ	-0.00065	0.06269	0.00000	0.37452	0.00000
16	O 2 S	-0.00047	0.37573	0.00000	-0.34022	0.00000
17	O 2 PX	0.00000	0.00000	0.21818	0.00000	0.00000
18	O 2 PY	0.00000	0.00000	0.00000	0.00000	0.46605
19	O 2 PZ	0.00009	0.02088	0.00000	0.33175	0.00000
20	O 2 DZ**2	-0.00002	0.00327	0.00000	0.01712	0.00000
21	O 2 DYY-ZZ	-0.00014	0.00739	0.00000	0.00483	0.00000
22	O 2 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
23	O 2 DXZ	0.00000	0.00000	0.02907	0.00000	0.00000
24	O 2 DYZ	0.00000	0.00000	0.00000	0.00000	0.01719
25	H 3 S	0.00020	0.09400	0.14839	0.08921	0.00000
26	H 3 S	0.00011	0.08124	0.21340	0.15338	0.00000
27	H 3 S	0.00009	-0.00244	0.05916	0.02886	0.00000
28	H 3 PX	-0.00008	-0.02346	-0.01818	-0.03082	0.00000
29	H 3 PY	0.00000	0.00000	0.00000	0.00000	0.03104
30	H 3 PZ	-0.00003	-0.01508	-0.02672	0.00771	0.00000

MO:			6	7	8	9	10
Eigenvalues:			0.14979	0.21729	0.56316	0.61934	0.99906
			A1	B1	B1	A1	A1
1	H	1 S	-0.03518	0.02677	-0.08420	0.06190	-0.03303
2	H	1 S	0.07062	-0.12332	-1.43073	1.82022	-0.61264
3	H	1 S	-0.83785	1.57295	0.75990	-0.62256	-0.09840
4	H	1 PX	0.00619	-0.00835	-0.02098	0.03177	-0.14895
5	H	1 PY	0.00000	0.00000	0.00000	0.00000	0.00000
6	H	1 PZ	0.00291	0.00852	-0.00360	-0.03801	0.11045
7	O	2 S	-0.03321	0.00000	0.00000	0.03375	-0.01513
8	O	2 S	-0.05414	0.00000	0.00000	0.05917	-0.02819
9	O	2 PX	0.00000	0.12342	-0.12106	0.00000	0.00000
10	O	2 PY	0.00000	0.00000	0.00000	0.00000	0.00000
11	O	2 PZ	0.07590	0.00000	0.00000	-0.10398	-0.23289
12	O	2 S	0.10255	0.00000	0.00000	-0.13690	0.06103
13	O	2 PX	0.00000	0.13237	-0.18251	0.00000	0.00000
14	O	2 PY	0.00000	0.00000	0.00000	0.00000	0.00000
15	O	2 PZ	0.11897	0.00000	0.00000	-0.19554	-0.73304
16	O	2 S	0.83473	0.00000	0.00000	-1.37814	0.94633
17	O	2 PX	0.00000	0.50248	-1.08125	0.00000	0.00000
18	O	2 PY	0.00000	0.00000	0.00000	0.00000	0.00000
19	O	2 PZ	0.21003	0.00000	0.00000	-1.08157	1.60243
20	O	2 DZ**2	0.00498	0.00000	0.00000	-0.01073	-0.00311
21	O	2 DYY-ZZ	0.00282	0.00000	0.00000	0.00943	0.01568
22	O	2 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
23	O	2 DXZ	0.00000	0.00479	0.01471	0.00000	0.00000
24	O	2 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
25	H	3 S	-0.03518	-0.02677	0.08420	0.06190	-0.03303
26	H	3 S	0.07062	0.12332	1.43073	1.82022	-0.61264
27	H	3 S	-0.83785	-1.57295	-0.75990	-0.62256	-0.09840
28	H	3 PX	-0.00619	-0.00835	-0.02098	-0.03177	0.14895
29	H	3 PY	0.00000	0.00000	0.00000	0.00000	0.00000
30	H	3 PZ	0.00291	-0.00852	0.00360	-0.03801	0.11045

MO:			11	12	13	14	15
Eigenvalues:			1.00320	1.11056	1.31556	1.45800	1.52184
			B2	B1	A1	A1	A2
1	H	1 S	0.00000	-0.01418	0.01278	0.08131	0.00000
2	H	1 S	0.00000	-0.33725	-0.88500	-1.16796	0.00000
3	H	1 S	0.00000	-0.78435	-0.33585	0.01804	0.00000
4	H	1 PX	0.00000	-0.16614	-0.14914	-0.60886	0.00000
5	H	1 PY	0.02020	0.00000	0.00000	0.00000	0.69071
6	H	1 PZ	0.00000	0.14814	0.37726	-0.38924	0.00000
7	O	2 S	0.00000	0.00000	0.09928	0.03509	0.00000
8	O	2 S	0.00000	0.00000	0.20427	0.07297	0.00000
9	O	2 PX	0.00000	0.24019	0.00000	0.00000	0.00000
10	O	2 PY	0.23996	0.00000	0.00000	0.00000	0.00000
11	O	2 PZ	0.00000	0.00000	-0.02928	0.01171	0.00000
12	O	2 S	0.00000	0.00000	-1.50196	-0.61744	0.00000
13	O	2 PX	0.00000	0.71715	0.00000	0.00000	0.00000
14	O	2 PY	0.83671	0.00000	0.00000	0.00000	0.00000
15	O	2 PZ	0.00000	0.00000	0.15834	0.10991	0.00000
16	O	2 S	0.00000	0.00000	3.13195	2.04767	0.00000
17	O	2 PX	0.00000	-1.78009	0.00000	0.00000	0.00000
18	O	2 PY	-1.15097	0.00000	0.00000	0.00000	0.00000
19	O	2 PZ	0.00000	0.00000	0.61973	1.24002	0.00000
20	O	2 DZ**2	0.00000	0.00000	0.03367	-0.10962	0.00000

21	O	2	DYY-ZZ	0.00000	0.00000	0.01471	0.05939	0.00000
22	O	2	DXY	0.00000	0.00000	0.00000	0.00000	-0.12479
23	O	2	DXZ	0.00000	-0.03011	0.00000	0.00000	0.00000
24	O	2	DYZ	0.00824	0.00000	0.00000	0.00000	0.00000
25	H	3	S	0.00000	0.01418	0.01278	0.08131	0.00000
26	H	3	S	0.00000	0.33725	-0.88500	-1.16796	0.00000
27	H	3	S	0.00000	0.78435	-0.33585	0.01804	0.00000
28	H	3	PX	0.00000	-0.16614	0.14914	0.60886	0.00000
29	H	3	PY	0.02020	0.00000	0.00000	0.00000	-0.69071
30	H	3	PZ	0.00000	-0.14814	0.37726	-0.38924	0.00000

MO:				16	17	18	19	20
Eigenvalues:				1.70567	1.93682	2.23909	2.39330	2.59470
				B2	B1	B1	A1	A1
1	H	1	S	0.00000	-0.19286	-0.67506	0.88727	0.55707
2	H	1	S	0.00000	0.74058	0.67504	-1.09387	-1.98125
3	H	1	S	0.00000	-0.16485	-0.53530	0.41175	0.26521
4	H	1	PX	0.00000	-0.48481	-0.29292	0.28841	-0.88058
5	H	1	PY	0.76517	0.00000	0.00000	0.00000	0.00000
6	H	1	PZ	0.00000	-0.65192	0.48640	-0.14126	0.68496
7	O	2	S	0.00000	0.00000	0.00000	0.03004	-0.05552
8	O	2	S	0.00000	0.00000	0.00000	0.05617	-0.12967
9	O	2	PX	0.00000	-0.01053	-0.17002	0.00000	0.00000
10	O	2	PY	-0.04918	0.00000	0.00000	0.00000	0.00000
11	O	2	PZ	0.00000	0.00000	0.00000	-0.16744	0.02276
12	O	2	S	0.00000	0.00000	0.00000	-0.24095	0.90481
13	O	2	PX	0.00000	-0.00869	-0.48123	0.00000	0.00000
14	O	2	PY	-0.05278	0.00000	0.00000	0.00000	0.00000
15	O	2	PZ	0.00000	0.00000	0.00000	-0.24415	0.68925
16	O	2	S	0.00000	0.00000	0.00000	0.13888	1.78476
17	O	2	PX	0.00000	0.88269	0.00364	0.00000	0.00000
18	O	2	PY	-0.55397	0.00000	0.00000	0.00000	0.00000
19	O	2	PZ	0.00000	0.00000	0.00000	0.23649	0.75532
20	O	2	DZ**2	0.00000	0.00000	0.00000	0.09033	-0.01256
21	O	2	DYY-ZZ	0.00000	0.00000	0.00000	0.27646	-0.00898
22	O	2	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
23	O	2	DXZ	0.00000	0.07493	0.23405	0.00000	0.00000
24	O	2	DYZ	0.14640	0.00000	0.00000	0.00000	0.00000
25	H	3	S	0.00000	0.19286	0.67506	0.88727	0.55707
26	H	3	S	0.00000	-0.74058	-0.67504	-1.09387	-1.98125
27	H	3	S	0.00000	0.16485	0.53530	0.41175	0.26521
28	H	3	PX	0.00000	-0.48481	-0.29292	-0.28841	0.88058
29	H	3	PY	0.76517	0.00000	0.00000	0.00000	0.00000
30	H	3	PZ	0.00000	0.65192	-0.48640	-0.14126	0.68496

MO:				21	22	23	24	25
Eigenvalues:				2.78656	3.50553	3.54430	3.72231	3.99864
				B1	B2	A2	A1	A1
1	H	1	S	-0.79018	0.00000	0.00000	-0.01712	0.31610
2	H	1	S	2.08233	0.00000	0.00000	-0.39987	1.09398
3	H	1	S	-0.52880	0.00000	0.00000	0.02542	0.04578
4	H	1	PX	0.90048	0.00000	0.00000	-0.34670	0.57430
5	H	1	PY	0.00000	0.36127	0.33765	0.00000	0.00000
6	H	1	PZ	-0.63450	0.00000	0.00000	-0.26543	-0.46534
7	O	2	S	0.00000	0.00000	0.00000	0.00053	0.02218
8	O	2	S	0.00000	0.00000	0.00000	0.00156	0.04406
9	O	2	PX	0.01179	0.00000	0.00000	0.00000	0.00000

10	O	2	PY	0.00000	-0.01983	0.00000	0.00000	0.00000
11	O	2	PZ	0.00000	0.00000	0.00000	0.03202	-0.30870
12	O	2	S	0.00000	0.00000	0.00000	-0.06757	-0.11846
13	O	2	PX	0.88076	0.00000	0.00000	0.00000	0.00000
14	O	2	PY	0.00000	0.01424	0.00000	0.00000	0.00000
15	O	2	PZ	0.00000	0.00000	0.00000	0.01207	-0.12952
16	O	2	S	0.00000	0.00000	0.00000	0.59744	-2.05336
17	O	2	PX	0.65083	0.00000	0.00000	0.00000	0.00000
18	O	2	PY	0.00000	-0.26991	0.00000	0.00000	0.00000
19	O	2	PZ	0.00000	0.00000	0.00000	0.55547	-0.99074
20	O	2	DZ**2	0.00000	0.00000	0.00000	1.06452	-0.19938
21	O	2	DYY-ZZ	0.00000	0.00000	0.00000	-0.21650	-1.09932
22	O	2	DXY	0.00000	0.00000	1.05209	0.00000	0.00000
23	O	2	DXZ	0.23174	0.00000	0.00000	0.00000	0.00000
24	O	2	DYZ	0.00000	-1.03612	0.00000	0.00000	0.00000
25	H	3	S	0.79018	0.00000	0.00000	-0.01712	0.31610
26	H	3	S	-2.08233	0.00000	0.00000	-0.39987	1.09398
27	H	3	S	0.52880	0.00000	0.00000	0.02542	0.04578
28	H	3	PX	0.90048	0.00000	0.00000	0.34670	-0.57430
29	H	3	PY	0.00000	0.36127	-0.33765	0.00000	0.00000
30	H	3	PZ	0.63450	0.00000	0.00000	-0.26543	-0.46534

MO:		26	27	28	29	30
Eigenvalues:		4.27434	5.32594	5.76281	6.17867	51.55007
		B1	B2	A1	B1	A1
1	H	1 S	0.40780	0.00000	0.28879	0.34577	-0.00560
2	H	1 S	0.50130	0.00000	0.49321	0.48971	-0.06533
3	H	1 S	0.23117	0.00000	0.01365	-0.15210	0.03041
4	H	1 PX	0.46086	0.00000	0.46235	0.50981	-0.05750
5	H	1 PY	0.00000	0.05881	0.00000	0.00000	0.00000
6	H	1 PZ	-0.36941	0.00000	-0.27987	-0.46713	0.04572
7	O	2 S	0.00000	0.00000	0.02261	0.00000	2.24716
8	O	2 S	0.00000	0.00000	0.04241	0.00000	-2.33609
9	O	2 PX	0.45261	0.00000	0.00000	-1.25404	0.00000
10	O	2 PY	0.00000	1.27047	0.00000	0.00000	0.00000
11	O	2 PZ	0.00000	0.00000	1.26271	0.00000	-0.01847
12	O	2 S	0.00000	0.00000	-0.22527	0.00000	0.26644
13	O	2 PX	-0.03633	0.00000	0.00000	1.98589	0.00000
14	O	2 PY	0.00000	-1.37394	0.00000	0.00000	0.00000
15	O	2 PZ	0.00000	0.00000	-1.72501	0.00000	0.07168
16	O	2 S	0.00000	0.00000	-1.01488	0.00000	-0.07433
17	O	2 PX	0.91370	0.00000	0.00000	-0.15896	0.00000
18	O	2 PY	0.00000	0.48123	0.00000	0.00000	0.00000
19	O	2 PZ	0.00000	0.00000	0.08461	0.00000	0.00932
20	O	2 DZ**2	0.00000	0.00000	-0.11479	0.00000	0.00419
21	O	2 DYY-ZZ	0.00000	0.00000	-0.35502	0.00000	0.02419
22	O	2 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
23	O	2 DXZ	1.15645	0.00000	0.00000	0.65292	0.00000
24	O	2 DYZ	0.00000	-0.02862	0.00000	0.00000	0.00000
25	H	3 S	-0.40780	0.00000	0.28879	-0.34577	-0.00560
26	H	3 S	-0.50130	0.00000	0.49321	-0.48971	-0.06533
27	H	3 S	-0.23117	0.00000	0.01365	0.15210	0.03041
28	H	3 PX	0.46086	0.00000	-0.46235	0.50981	0.05750
29	H	3 PY	0.00000	0.05881	0.00000	0.00000	0.00000
30	H	3 PZ	0.36941	0.00000	-0.27987	0.46713	0.04572

Dipole moment: X = 0.000000 Y = 0.000000 Z = 2.195271
Total Dipole: 2.195271 Debye

```
 Atomic Charges from Electrostatic Potential

 Resolution:   1  points per atomic unit

  2541 of   6137 gridpoints used in calculation


    Atom     Charge
    ----   -----------

    H  1     0.388060
    O  2    -0.776119
    H  3     0.388060

 Total Charge =  0.000000


 RMS fit:    1.086187
 RRMS fit:   0.107225


 Dipole moment from formal charges:

 x =   0.0000, y =   0.0000, z =   2.2329  =   2.2329 debye

Q-minus(elesta) =  -0.7761
Q-plus(elesta)  =   0.3881

 Mulliken Population Analysis

   AO  ATOM      Occupancy
   --  ----      ---------

    1     1       0.266413
    2     1       0.387656
    3     1       0.029492
    4     1       0.027473
    5     1       0.021559
    6     1       0.021824
    7     2       1.083494
    8     2       0.912344
    9     2       0.248847
   10     2       0.383572
   11     2       0.304211
   12     2       0.985530
   13     2       0.593756
   14     2       0.807522
   15     2       0.672125
   16     2       0.801353
   17     2       0.368406
   18     2       0.764808
   19     2       0.552710
   20     2       0.001378
   21     2       0.001206
   22     2       0.000000
   23     2       0.008926
   24     2       0.000980
   25     3       0.266413
   26     3       0.387656
   27     3       0.029492
   28     3       0.027473
```

```
  29     3       0.021559
  30     3       0.021824

   Atom    Occupancy      Charge
   ----   -----------  -----------

   H  1     0.754416     0.245584
   O  2     8.491168    -0.491168
   H  3     0.754416     0.245584

 Total Charge =  0.000000


 Natural Atomic Orbital Populations

 Nao  Atom   Type   Basis  Occupancy
 ---  ----  ------- -----  ---------

   1  H  1  S        MIN    0.550092
   2  H  1  S        RYD    0.002180
   3  H  1  S        RYD    0.000066
   4  H  1  PX       RYD    0.000840
   5  H  1  PY       RYD    0.001326
   6  H  1  PZ       RYD    0.000887
   7  O  2  S        MIN    1.999856
   8  O  2  S        MIN    1.744914
   9  O  2  S        RYD    0.000587
  10  O  2  S        RYD    0.000000
  11  O  2  PX       MIN    1.439373
  12  O  2  PX       RYD    0.001868
  13  O  2  PX       RYD    0.000000
  14  O  2  PY       MIN    1.995258
  15  O  2  PY       RYD    0.000811
  16  O  2  PY       RYD    0.000000
  17  O  2  PZ       MIN    1.698246
  18  O  2  PZ       RYD    0.000099
  19  O  2  PZ       RYD    0.000021
  20  O  2  DXY      RYD    0.000000
  21  O  2  DXZ      RYD    0.004241
  22  O  2  DYZ      RYD    0.001279
  23  O  2  DXX-YY   RYD    0.001006
  24  O  2  D3ZZ-RR  RYD    0.001657
  25  H  3  S        MIN    0.550092
  26  H  3  S        RYD    0.002180
  27  H  3  S        RYD    0.000066
  28  H  3  PX       RYD    0.000840
  29  H  3  PY       RYD    0.001326
  30  H  3  PZ       RYD    0.000887

 Total MIN occupancy:   9.977831
 Total RYD occupancy:   0.022169
 Total occupancy:      10.000000


 Natural Atomic Populations and Charges

  Atom    Occupancy     Charge
  ----   -----------  -----------

  H  1     0.555392     0.444608
  O  2     8.889217    -0.889217
```

```
   H  3     0.555392     0.444608

  Total Charge =  0.000000

Q-minus(NAO) =  -0.8892
Q-plus(NAO)  =   0.4446


  Mulliken Bond Order Matrix

            1         2

   2     0.96330
   3     0.00636   0.96330


   Atomic Valencies

     Atom      Valency
     ----      -------

     H   1     0.969659
     O   2     1.926595
     H   3     0.969659

  Lowdin Bond Order Matrix

            1         2

   2     1.17929
   3     0.06914   1.17929


   Atomic Valencies

     Atom      Valency
     ----      -------

     H   1     1.248433
     O   2     2.358589
     H   3     1.248433

  Frequencies and reduced mass in atomic units are:

 mode     (cm-1)         AU          mass
    1   -0.3317E-04  -0.4163E-16  -0.4532E+16
    2   -0.1808E-04  -0.1236E-16  -0.2275E+17
    3   -0.1796E-12  -0.1221E-32   0.5948E+28
    4   -0.9515E-13  -0.3426E-33   0.6255E+28
    5    0.1739E-04   0.1145E-16   0.2018E+17
    6    0.2753E-04   0.2868E-16   0.1139E+16
    7     1667.       0.1052        1.892
    8     3910.       0.5785       0.8373
    9     4018.       0.6108        1.037

  Zero-point vibrational energy is    13.716 kcal/mol

  Standard Thermodynamic quantities at   298.15 K  and     1.00 atm

  Translational Enthalpy:        0.889 kcal/mol
  Rotational Enthalpy:           0.889 kcal/mol
```

```
  Vibrational Enthalpy:         13.718 kcal/mol

  Translational Entropy:        34.608  cal/mol.K
  Rotational Entropy:           10.461  cal/mol.K
  Vibrational Entropy:           0.006  cal/mol.K

  Total Cpu time:   0 mins.  1.22 secs.

SPARTAN GRAPHICS PROGRAM:  SGI/R5K        Release 5.0.1
  (Job run on newton)

Graphics requests:

surface=density value=0.002 property=homo-1 resolution=med  pending

surface=density value=0.002 property=homo resolution=med  pending

surface=density value=0.002 property=homo-2 resolution=med  pending

surface=density value=0.002 property=homo-3 resolution=med  pending

surface=density value=0.002 property=homo-4 resolution=med  pending

volume=homo x=-2.10~2.10 y=-2.10~2.10 z=-1.82~2.38 resolution=med  pending

volume=homo-1 x=-2.10~2.10 y=-2.10~2.10 z=-1.82~2.38 resolution=med  pending

volume=homo-2 x=-2.10~2.10 y=-2.10~2.10 z=-1.82~2.38 resolution=med  pending

volume=homo-3 x=-2.10~2.10 y=-2.10~2.10 z=-1.82~2.38 resolution=med  pending

volume=homo-4 x=-2.10~2.10 y=-2.10~2.10 z=-1.82~2.38 resolution=med  pending


Graphics files written:

gr_request.2

gr_request.3

gr_request.4

gr_request.5

gr_request.6

gr_request.1

gr_request.7

gr_request.8

gr_request.9

gr_request.10

Surface    Type        Property    S.mo P.mo Resolution  Value   Size

    1     Density         MO               4    0.500    0.002  2.000
```

2	Density	MO	5	0.500	0.002	2.000
3	Density	MO	3	0.500	0.002	2.000
4	Density	MO	2	0.500	0.002	2.000
5	Density	MO	1	0.500	0.002	2.000
6	MO	5		0.500	0.032	2.000
7	MO	4		0.500	0.032	2.000
8	MO	3		0.500	0.032	2.000
9	MO	2		0.500	0.032	2.000
10	MO	1		0.500	0.032	2.000

Calculation required 0 mins. 3.89 seconds

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:05:10 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   2
     2 S shells
  Number of basis functions:   2
  Number of electrons:   1
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    H  H2          -0.0000001     0.7248522    -3.1082902

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.12E-05 in   5 cycles  <S**2> = 0.7500

  E(HF)  =      -0.4961985 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1          2

  Eigenvalues:       -0.49620    1.06900

                        A          A
   1 H   1 S          0.37327    1.25558
   2 H   1 S          0.71744   -1.09594

  Beta Spin Molecular Orbital Coefficients

  MO:                   1          2

  Eigenvalues:        0.11335    1.25770

                        A          A
   1 H   1 S          0.16409    1.29957
   2 H   1 S          0.88614   -0.96466

    ** Archive file written to unit 12 **

  Total Cpu time:         0 mins.  0.14 secs.
  Total Wall time:        0 mins.  1.98 secs.

  Calculation finished: Fri Sep 18 13:05:12 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
```

```
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.02 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:18:26 1998

  Run type: Single point energy
  Model: RHF/STO-3G
  Number of shells:   1
     1 S shells
  Number of basis functions:   1
  Number of electrons:   2
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    He He1          0.0000000     2.2781070    -2.8971898

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  RHF direct SCF procedure requested

  Energy converged to 0.00E+00 in   2 cycles

  E(HF)  =      -2.8077840 a.u.

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1

  Eigenvalues:      -0.87604

                        A
   1 He  1 S         1.00000

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  0.02 secs.
  Total Wall time:       0 mins.  0.22 secs.

  Calculation finished: Fri Sep 18 13:18:26 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.02 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:18:57 1998

  Run type: Single point energy
  Model: UHF/STO-3G
  Number of shells:   1
     1 S shells
  Number of basis functions:   1
  Number of electrons:   1
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    He He1         -0.0000001     2.2781070    -2.8971898

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to 0.00E+00 in   2 cycles  <S**2> = 0.7500

  E(HF)  =      -1.9317484 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1

  Eigenvalues:      -1.93175

                        A
   1 He  1 S         1.00000

  Beta Spin Molecular Orbital Coefficients

  MO:                   1

  Eigenvalues:      -0.87604

                        A
   1 He  1 S         1.00000

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  0.02 secs.
  Total Wall time:       0 mins.  0.16 secs.

  Calculation finished: Fri Sep 18 13:18:57 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis
```

```
 Total Cpu time:   0 mins.  0.02 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:16:09 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   3
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Li Li1          0.0000000     3.4792904    -2.1635387

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.25E-07 in   5 cycles  <S**2> = 0.7500

  E(HF)  =      -7.3815132 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:      -2.46050   -0.19443    0.02644    0.02644    0.02644

                        A          A          A          A          A
   1 Li  1 S        -0.99122   -0.19624    0.00000    0.00000    0.00000
   2 Li  1 S        -0.06317    0.37522    0.00000    0.00000    0.00000
   3 Li  1 PX        0.00000    0.00000   -0.01039   -0.04700   -0.18705
   4 Li  1 PY        0.00000    0.00000    0.13820   -0.13248    0.02561
   5 Li  1 PZ        0.00000    0.00000   -0.13453   -0.13246    0.04076
   6 Li  1 S         0.02461    0.69181    0.00000    0.00000    0.00000
   7 Li  1 PX        0.00000    0.00000   -0.04703   -0.21270   -0.84647
   8 Li  1 PY        0.00000    0.00000    0.62540   -0.59951    0.11589
   9 Li  1 PZ        0.00000    0.00000   -0.60880   -0.59943    0.18445

  MO:                   6          7          8          9

  Eigenvalues:       0.16885    0.19741    0.19741    0.19741

                        A          A          A          A
   1 Li  1 S         0.10684    0.00000    0.00000    0.00000
   2 Li  1 S        -1.57115    0.00000    0.00000    0.00000
   3 Li  1 PX        0.00000   -0.04502   -1.18701   -0.28595
   4 Li  1 PY        0.00000   -1.02690    0.19160   -0.63369
   5 Li  1 PZ        0.00000   -0.66049   -0.21698    1.00472
```

6 Li	1 S	1.45021	0.00000	0.00000	0.00000
7 Li	1 PX	0.00000	0.03225	0.85036	0.20485
8 Li	1 PY	0.00000	0.73566	-0.13726	0.45397
9 Li	1 PZ	0.00000	0.47317	0.15544	-0.71977

Beta Spin Molecular Orbital Coefficients

MO:		1	2	3	4	5
Eigenvalues:		-2.44386	0.02162	0.05735	0.05735	0.05735
		A	A	A	A	A
1 Li	1 S	0.99074	0.16032	0.00000	0.00000	0.00000
2 Li	1 S	0.06598	0.07299	0.00000	0.00000	0.00000
3 Li	1 PX	0.00000	0.00000	-0.01082	-0.01797	-0.02424
4 Li	1 PY	0.00000	0.00000	-0.03014	0.00762	0.00781
5 Li	1 PZ	0.00000	0.00000	-0.00138	-0.02543	0.01947
6 Li	1 S	-0.02549	-1.06517	0.00000	0.00000	0.00000
7 Li	1 PX	0.00000	0.00000	-0.33110	-0.54987	-0.74161
8 Li	1 PY	0.00000	0.00000	-0.92225	0.23310	0.23892
9 Li	1 PZ	0.00000	0.00000	-0.04230	-0.77799	0.59574

MO:		6	7	8	9
Eigenvalues:		0.21825	0.22849	0.22849	0.22849
		A	A	A	A
1 Li	1 S	0.15863	0.00000	0.00000	0.00000
2 Li	1 S	-1.61357	0.00000	0.00000	0.00000
3 Li	1 PX	0.00000	-0.17318	-1.20785	0.20042
4 Li	1 PY	0.00000	1.08088	-0.05573	0.59805
5 Li	1 PZ	0.00000	0.57513	-0.25894	-1.06359
6 Li	1 S	1.20294	0.00000	0.00000	0.00000
7 Li	1 PX	0.00000	0.10556	0.73624	-0.12217
8 Li	1 PY	0.00000	-0.65885	0.03397	-0.36454
9 Li	1 PZ	0.00000	-0.35057	0.15784	0.64831

** Archive file written to unit 12 **

Total Cpu time: 0 mins. 0.21 secs.
Total Wall time: 0 mins. 0.45 secs.

Calculation finished: Fri Sep 18 13:16:10 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

Total Cpu time: 0 mins. 0.03 secs.

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:13:13 1998

  Run type: Single point energy
  Model: RHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   4
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Be Be1          0.0000000     2.8372787    -2.4822491

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  RHF direct SCF procedure requested

  Energy converged to -.22E-07 in   5 cycles

  E(HF)  =     -14.4868202 a.u.

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:       -4.68838   -0.30564    0.07141    0.07141    0.07141

                        A          A          A          A          A
   1 Be  1 S          0.99281    0.21571    0.00000    0.00000    0.00000
   2 Be  1 S          0.07643   -0.22934    0.00000    0.00000    0.00000
   3 Be  1 PX         0.00000    0.00000   -0.01217   -0.00409   -0.25643
   4 Be  1 PY         0.00000    0.00000   -0.16072    0.20017    0.00443
   5 Be  1 PZ         0.00000    0.00000    0.19985    0.16073   -0.01205
   6 Be  1 S         -0.02873   -0.82235    0.00000    0.00000    0.00000
   7 Be  1 PX         0.00000    0.00000   -0.03919   -0.01318   -0.82606
   8 Be  1 PY         0.00000    0.00000   -0.51774    0.64485    0.01427
   9 Be  1 PZ         0.00000    0.00000    0.64381    0.51777   -0.03881

  MO:                   6          7          8          9

  Eigenvalues:        0.46420    0.46420    0.46420    0.55261

                        A          A          A          A
   1 Be  1 S          0.00000    0.00000    0.00000    0.01378
   2 Be  1 S          0.00000    0.00000    0.00000   -1.64476
   3 Be  1 PX        -0.11034    0.22689    1.18348    0.00000
   4 Be  1 PY         0.50997    1.08555   -0.16057    0.00000
   5 Be  1 PZ        -1.09180    0.48412   -0.19460    0.00000
```

```
   6 Be  1 S         0.00000    0.00000    0.00000    1.45604
   7 Be  1 PX        0.08387   -0.17247   -0.89962    0.00000
   8 Be  1 PY       -0.38765   -0.82518    0.12206    0.00000
   9 Be  1 PZ        0.82993   -0.36800    0.14793    0.00000

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  0.20 secs.
  Total Wall time:       0 mins.  1.53 secs.

  Calculation finished: Fri Sep 18 13:13:14 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.02 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:11:22 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   5
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    B  B1           0.0000000    -2.6923087     4.3283113

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.31E-10 in   9 cycles  <S**2> = 0.7503

  E(HF)  =     -24.3897617 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:      -7.64805   -0.53690   -0.30716    0.06339    0.06339

                        A          A          A          A          A
   1 B   1 S         0.98797    0.23188    0.00000    0.00000    0.00000
   2 B   1 S         0.08098   -0.30195    0.00000    0.00000    0.00000
   3 B   1 PX        0.00000    0.00000   -0.50278    0.13151    0.03438
   4 B   1 PY        0.00000    0.00000   -0.09745   -0.07605   -0.34926
   5 B   1 PZ        0.00000    0.00000   -0.17786   -0.33008    0.09417
   6 B   1 S        -0.02689   -0.76444    0.00000    0.00000    0.00000
   7 B   1 PX        0.00000    0.00000   -0.54994    0.27239    0.07121
   8 B   1 PY        0.00000    0.00000   -0.10659   -0.15753   -0.72342
   9 B   1 PZ        0.00000    0.00000   -0.19454   -0.68369    0.19505

  MO:                   6          7          8          9

  Eigenvalues:       0.59801    0.65930    0.65930    0.77720

                        A          A          A          A
   1 B   1 S         0.00000    0.00000    0.00000   -0.08667
   2 B   1 S         0.00000    0.00000    0.00000    1.55699
   3 B   1 PX       -0.99134   -0.34144    0.25686    0.00000
   4 B   1 PY       -0.19215    1.00891    0.49446    0.00000
   5 B   1 PZ       -0.35069    0.41239   -0.99703    0.00000
```

```
  6 B   1 S         0.00000    0.00000    0.00000   -1.38871
  7 B   1 PX        0.96598    0.27885   -0.20978    0.00000
  8 B   1 PY        0.18723   -0.82398   -0.40383    0.00000
  9 B   1 PZ        0.34172   -0.33680    0.81427    0.00000

  Beta Spin Molecular Orbital Coefficients

  MO:                  1          2          3          4          5

  Eigenvalues:      -7.63435   -0.44090    0.08471    0.08471    0.12748

                       A          A          A          A          A
  1 B   1 S         0.98863    0.22792    0.00000    0.00000    0.00000
  2 B   1 S         0.07839   -0.27466    0.00000    0.00000    0.00000
  3 B   1 PX        0.00000    0.00000   -0.12845   -0.01504   -0.29806
  4 B   1 PY        0.00000    0.00000    0.18827   -0.28323   -0.05777
  5 B   1 PZ        0.00000    0.00000    0.25996    0.19769   -0.10544
  6 B   1 S        -0.02711   -0.78873    0.00000    0.00000    0.00000
  7 B   1 PX        0.00000    0.00000   -0.28494   -0.03336   -0.72912
  8 B   1 PY        0.00000    0.00000    0.41764   -0.62827   -0.14132
  9 B   1 PZ        0.00000    0.00000    0.57666    0.43853   -0.25793

  MO:                  6          7          8          9

  Eigenvalues:       0.67356    0.67356    0.71458    0.81020

                       A          A          A          A
  1 B   1 S         0.00000    0.00000    0.00000    0.08953
  2 B   1 S         0.00000    0.00000    0.00000   -1.56217
  3 B   1 PX        0.25645   -0.34430   -1.07084    0.00000
  4 B   1 PY        0.50167    1.01135   -0.20755    0.00000
  5 B   1 PZ       -0.99981    0.41915   -0.37881    0.00000
  6 B   1 S         0.00000    0.00000    0.00000    1.37506
  7 B   1 PX       -0.20583    0.27634    0.83901    0.00000
  8 B   1 PY       -0.40265   -0.81172    0.16262    0.00000
  9 B   1 PZ        0.80246   -0.33641    0.29680    0.00000

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  0.12 secs.
  Total Wall time:       0 mins.  0.31 secs.

  Calculation finished: Fri Sep 18 13:11:22 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.03 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 12:47:21 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   6
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  3

                     Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    C  C1          -0.0000001     2.1124265    -3.4283320

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.72E-05 in   5 cycles  <S**2> = 2.0010

  E(HF)  =     -37.4810698 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:     -11.27249   -0.81445   -0.42596   -0.42596    0.05295

                        A          A          A          A          A
   1 C   1 S         0.98568    0.24488    0.00000    0.00000    0.00000
   2 C   1 S         0.08664   -0.28976    0.00000    0.00000    0.00000
   3 C   1 PX        0.00000    0.00000    0.38429   -0.40249    0.00000
   4 C   1 PY        0.00000    0.00000   -0.40249   -0.38429    0.00000
   5 C   1 PZ        0.00000    0.00000    0.00000    0.00000   -0.41040
   6 C   1 S        -0.02549   -0.77978    0.00000    0.00000    0.00000
   7 C   1 PX        0.00000    0.00000    0.40543   -0.42464    0.00000
   8 C   1 PY        0.00000    0.00000   -0.42464   -0.40543    0.00000
   9 C   1 PZ        0.00000    0.00000    0.00000    0.00000   -0.72030

  MO:                   6          7          8          9

  Eigenvalues:       0.89799    0.89799    0.97612    1.24659

                        A          A          A          A
   1 C   1 S         0.00000    0.00000    0.00000    0.09788
   2 C   1 S         0.00000    0.00000    0.00000   -1.51818
   3 C   1 PX        0.81005    0.65011    0.00000    0.00000
   4 C   1 PY       -0.65011    0.81005    0.00000    0.00000
   5 C   1 PZ        0.00000    0.00000   -1.10457    0.00000
```

```
  6 C   1 S         0.00000    0.00000    0.00000    1.33319
  7 C   1 PX       -0.79680   -0.63947    0.00000    0.00000
  8 C   1 PY        0.63947   -0.79680    0.00000    0.00000
  9 C   1 PZ        0.00000    0.00000    0.93256    0.00000

  Beta Spin Molecular Orbital Coefficients

  MO:                  1          2          3          4          5

  Eigenvalues:    -11.23139   -0.57527    0.10809    0.16273    0.16273

                       A          A          A          A          A
  1 C   1 S         0.98704    0.23720    0.00000    0.00000    0.00000
  2 C   1 S         0.08174   -0.24285    0.00000    0.00000    0.00000
  3 C   1 PX        0.00000    0.00000    0.00000   -0.02030   -0.36119
  4 C   1 PY        0.00000    0.00000    0.00000    0.36119   -0.02030
  5 C   1 PZ        0.00000    0.00000    0.38229    0.00000    0.00000
  6 C   1 S        -0.02602   -0.82070    0.00000    0.00000    0.00000
  7 C   1 PX        0.00000    0.00000    0.00000   -0.04267   -0.75915
  8 C   1 PY        0.00000    0.00000    0.00000    0.75915   -0.04267
  9 C   1 PZ        0.00000    0.00000    0.74369    0.00000    0.00000

  MO:                  6          7          8          9

  Eigenvalues:      1.01164    1.06360    1.06360    1.33242

                       A          A          A          A
  1 C   1 S         0.00000    0.00000    0.00000   -0.10300
  2 C   1 S         0.00000    0.00000    0.00000    1.52666
  3 C   1 PX        0.00000    0.76110   -0.82362    0.00000
  4 C   1 PY        0.00000   -0.82362   -0.76110    0.00000
  5 C   1 PZ       -1.11461    0.00000    0.00000    0.00000
  6 C   1 S         0.00000    0.00000    0.00000   -1.30839
  7 C   1 PX        0.00000   -0.61095    0.66114    0.00000
  8 C   1 PY        0.00000    0.66114    0.61095    0.00000
  9 C   1 PZ        0.91401    0.00000    0.00000    0.00000

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  0.20 secs.
  Total Wall time:       0 mins.  2.32 secs.

  Calculation finished: Fri Sep 18 12:47:24 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.03 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:20:26 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   7
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  4

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    N  N1          -0.0000001     1.3875744    -2.9318705

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.14E-06 in   6 cycles  <S**2> = 3.7516

  E(HF)  =     -54.1053904 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:     -15.57262   -1.14139   -0.55386   -0.55386   -0.55386

                        A          A          A          A          A
   1 N   1 S         -0.98388   -0.25343    0.00000    0.00000    0.00000
   2 N   1 S         -0.09214    0.27933    0.00000    0.00000    0.00000
   3 N   1 PX         0.00000    0.00000   -0.10419   -0.42677   -0.35230
   4 N   1 PY         0.00000    0.00000    0.05707    0.34829   -0.43879
   5 N   1 PZ         0.00000    0.00000    0.55044   -0.11689   -0.02119
   6 N   1 S          0.02487    0.79159    0.00000    0.00000    0.00000
   7 N   1 PX         0.00000    0.00000   -0.10832   -0.44366   -0.36624
   8 N   1 PY         0.00000    0.00000    0.05933    0.36207   -0.45616
   9 N   1 PZ         0.00000    0.00000    0.57223   -0.12152   -0.02203

  MO:                   6          7          8          9

  Eigenvalues:       1.26027    1.26027    1.26027    1.83427

                        A          A          A          A
   1 N   1 S         0.00000    0.00000    0.00000   -0.10382
   2 N   1 S         0.00000    0.00000    0.00000    1.49469
   3 N   1 PX       -0.96280    0.31622    0.13706    0.00000
   4 N   1 PY       -0.30350   -0.97063    0.10742    0.00000
   5 N   1 PZ        0.16331    0.06046    1.00770    0.00000
```

```
  6 N   1 S         0.00000    0.00000    0.00000   -1.29755
  7 N   1 PX        0.95095   -0.31233   -0.13537    0.00000
  8 N   1 PY        0.29976    0.95868   -0.10609    0.00000
  9 N   1 PZ       -0.16130   -0.05971   -0.99529    0.00000

  Beta Spin Molecular Orbital Coefficients

  MO:                  1          2          3          4          5

  Eigenvalues:     -15.49032   -0.71462    0.19985    0.19985    0.19985

                       A          A          A          A          A
  1 N   1 S        -0.98584   -0.24283    0.00000    0.00000    0.00000
  2 N   1 S        -0.08537    0.22003    0.00000    0.00000    0.00000
  3 N   1 PX        0.00000    0.00000    0.37681   -0.09019   -0.02447
  4 N   1 PY        0.00000    0.00000    0.09299    0.37200    0.06073
  5 N   1 PZ        0.00000    0.00000    0.00934   -0.06480    0.38267
  6 N   1 S         0.02570    0.84257    0.00000    0.00000    0.00000
  7 N   1 PX        0.00000    0.00000    0.72092   -0.17256   -0.04681
  8 N   1 PY        0.00000    0.00000    0.17790    0.71172    0.11619
  9 N   1 PZ        0.00000    0.00000    0.01787   -0.12399    0.73212

  MO:                  6          7          8          9

  Eigenvalues:       1.47982    1.47982    1.47982    1.99176

                       A          A          A          A
  1 N   1 S         0.00000    0.00000    0.00000   -0.11034
  2 N   1 S         0.00000    0.00000    0.00000    1.50496
  3 N   1 PX       -0.73536    0.81504   -0.08425    0.00000
  4 N   1 PY       -0.80878   -0.74015   -0.10100    0.00000
  5 N   1 PZ        0.13141    0.00557   -1.09309    0.00000
  6 N   1 S         0.00000    0.00000    0.00000   -1.26502
  7 N   1 PX        0.60156   -0.66675    0.06892    0.00000
  8 N   1 PY        0.66162    0.60548    0.08263    0.00000
  9 N   1 PZ       -0.10750   -0.00456    0.89421    0.00000

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  0.22 secs.
  Total Wall time:       0 mins.  0.98 secs.

  Calculation finished: Fri Sep 18 13:20:27 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.03 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:23:18 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   8
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  3

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    O  O1           0.0000000     3.2307700    -2.0269174

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.24E-05 in   6 cycles  <S**2> = 2.0011

  E(HF)  =     -74.3936572 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:     -20.57421   -1.37752   -0.67294   -0.67294   -0.58558

                        A          A          A          A          A
   1 O   1 S         0.98221   -0.25743    0.00000    0.00000    0.00000
   2 O   1 S         0.09243    0.27963    0.00000    0.00000    0.00000
   3 O   1 PX        0.00000    0.00000    0.00000    0.00000    0.55965
   4 O   1 PY        0.00000    0.00000   -0.47546    0.32020    0.00000
   5 O   1 PZ        0.00000    0.00000    0.32020    0.47546    0.00000
   6 O   1 S        -0.02385    0.79477    0.00000    0.00000    0.00000
   7 O   1 PX        0.00000    0.00000    0.00000    0.00000    0.59535
   8 O   1 PY        0.00000    0.00000   -0.48269    0.32506    0.00000
   9 O   1 PZ        0.00000    0.00000    0.32506    0.48269    0.00000

  MO:                   6          7          8          9

  Eigenvalues:       1.62944    1.62944    1.69854    2.42707

                        A          A          A          A
   1 O   1 S         0.00000    0.00000    0.00000   -0.12923
   2 O   1 S         0.00000    0.00000    0.00000    1.46685
   3 O   1 PX        0.00000    0.00000   -1.00893    0.00000
   4 O   1 PY       -0.99393   -0.12107    0.00000    0.00000
   5 O   1 PZ       -0.12107    0.99393    0.00000    0.00000
```

6	O	1	S	0.00000	0.00000	0.00000	-1.25794
7	O	1	PX	0.00000	0.00000	0.98829	0.00000
8	O	1	PY	0.98893	0.12047	0.00000	0.00000
9	O	1	PZ	0.12047	-0.98893	0.00000	0.00000

Beta Spin Molecular Orbital Coefficients

MO:				1	2	3	4	5
Eigenvalues:				-20.50307	-1.04820	-0.49181	0.17155	0.17155
				A	A	A	A	A
1	O	1	S	0.98351	-0.25019	0.00000	0.00000	0.00000
2	O	1	S	0.08816	0.24291	0.00000	0.00000	0.00000
3	O	1	PX	0.00000	0.00000	0.53791	0.00000	0.00000
4	O	1	PY	0.00000	0.00000	0.00000	-0.01659	0.42739
5	O	1	PZ	0.00000	0.00000	0.00000	-0.42739	-0.01659
6	O	1	S	-0.02435	0.82614	0.00000	0.00000	0.00000
7	O	1	PX	0.00000	0.00000	0.61637	0.00000	0.00000
8	O	1	PY	0.00000	0.00000	0.00000	-0.02775	0.71488
9	O	1	PZ	0.00000	0.00000	0.00000	-0.71488	-0.02775

MO:				6	7	8	9
Eigenvalues:				1.75008	1.86132	1.86132	2.55158
				A	A	A	A
1	O	1	S	0.00000	0.00000	0.00000	-0.13347
2	O	1	S	0.00000	0.00000	0.00000	1.47364
3	O	1	PX	-1.02068	0.00000	0.00000	0.00000
4	O	1	PY	0.00000	-1.05263	0.20045	0.00000
5	O	1	PZ	0.00000	0.20045	1.05263	0.00000
6	O	1	S	0.00000	0.00000	0.00000	-1.23755
7	O	1	PX	0.97531	0.00000	0.00000	0.00000
8	O	1	PY	0.00000	0.88919	-0.16932	0.00000
9	O	1	PZ	0.00000	-0.16932	-0.88919	0.00000

** Archive file written to unit 12 **

Total Cpu time: 0 mins. 0.21 secs.
Total Wall time: 0 mins. 0.58 secs.

Calculation finished: Fri Sep 18 13:23:18 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

Total Cpu time: 0 mins. 0.03 secs.

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:24:54 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   9
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    F  F1          -0.0000001     0.7455622    -1.5089561

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.18E-05 in   6 cycles  <S**2> = 0.7503

  E(HF)  =     -98.8450093 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:     -26.23761   -1.61823   -0.78885   -0.68908   -0.68908

                        A          A          A          A          A
   1 F   1 S         0.98135   -0.25938    0.00000    0.00000    0.00000
   2 F   1 S         0.09322    0.26896    0.00000    0.00000    0.00000
   3 F   1 PX        0.00000    0.00000    0.00000    0.06996    0.55781
   4 F   1 PY        0.00000    0.00000    0.00000   -0.55781    0.06996
   5 F   1 PZ        0.00000    0.00000    0.57474    0.00000    0.00000
   6 F   1 S        -0.02328    0.80601    0.00000    0.00000    0.00000
   7 F   1 PX        0.00000    0.00000    0.00000    0.07427    0.59221
   8 F   1 PY        0.00000    0.00000    0.00000   -0.59221    0.07427
   9 F   1 PZ        0.00000    0.00000    0.58445    0.00000    0.00000

  MO:                   6          7          8          9

  Eigenvalues:       2.08165    2.16083    2.16083    3.19452

                        A          A          A          A
   1 F   1 S         0.00000    0.00000    0.00000   -0.14020
   2 F   1 S         0.00000    0.00000    0.00000    1.45124
   3 F   1 PX        0.00000   -0.26837    0.96184    0.00000
   4 F   1 PY        0.00000   -0.96184   -0.26837    0.00000
   5 F   1 PZ       -0.99140    0.00000    0.00000    0.00000
```

```
  6 F   1 S         0.00000    0.00000    0.00000   -1.22836
  7 F   1 PX        0.00000    0.26291   -0.94226    0.00000
  8 F   1 PY        0.00000    0.94226    0.26291    0.00000
  9 F   1 PZ        0.98571    0.00000    0.00000    0.00000

  Beta Spin Molecular Orbital Coefficients

  MO:                  1          2          3          4          5

  Eigenvalues:    -26.19418   -1.43150   -0.63588   -0.63588    0.13450

                       A          A          A          A          A
  1 F   1 S         0.98197    0.25594    0.00000    0.00000    0.00000
  2 F   1 S         0.09123   -0.25251    0.00000    0.00000    0.00000
  3 F   1 PX        0.00000    0.00000    0.10893    0.54194    0.00000
  4 F   1 PY        0.00000    0.00000   -0.54194    0.10893    0.00000
  5 F   1 PZ        0.00000    0.00000    0.00000    0.00000   -0.45468
  6 F   1 S        -0.02351   -0.81996    0.00000    0.00000    0.00000
  7 F   1 PX        0.00000    0.00000    0.11942    0.59412    0.00000
  8 F   1 PY        0.00000    0.00000   -0.59412    0.11942    0.00000
  9 F   1 PZ        0.00000    0.00000    0.00000    0.00000   -0.69587

  MO:                  6          7          8          9

  Eigenvalues:      2.18976    2.18976    2.31792    3.26643

                       A          A          A          A
  1 F   1 S         0.00000    0.00000    0.00000   -0.14213
  2 F   1 S         0.00000    0.00000    0.00000    1.45432
  3 F   1 PX        0.06139    1.00193    0.00000    0.00000
  4 F   1 PY       -1.00193    0.06139    0.00000    0.00000
  5 F   1 PZ        0.00000    0.00000   -1.05189    0.00000
  6 F   1 S         0.00000    0.00000    0.00000   -1.21909
  7 F   1 PX       -0.05948   -0.97079    0.00000    0.00000
  8 F   1 PY        0.97079   -0.05948    0.00000    0.00000
  9 F   1 PZ        0.00000    0.00000    0.91048    0.00000

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  0.21 secs.
  Total Wall time:       0 mins.  0.54 secs.

  Calculation finished: Fri Sep 18 13:24:55 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.03 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:28:35 1998

  Run type: Single point energy
  Model: RHF/STO-3G
  Number of shells:   2
     1 S shells
     1 SP shells
  Number of basis functions:   5
  Number of electrons:  10
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Ne Ne1         -0.0000001     0.7041422    -3.4763319

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  RHF direct SCF procedure requested

  Energy converged to 0.00E+00 in   2 cycles

  E(HF)  =    -126.6045251 a.u.

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:     -32.21252   -1.70610   -0.54305   -0.54305   -0.54305

                        A          A          A          A          A
   1 Ne  1 S         -0.99501   -0.26941    0.00000    0.00000    0.00000
   2 Ne  1 S         -0.01978    1.03065    0.00000    0.00000    0.00000
   3 Ne  1 PX         0.00000    0.00000    0.00000   -0.81407   -0.58077
   4 Ne  1 PY         0.00000    0.00000    0.00040   -0.58077    0.81407
   5 Ne  1 PZ         0.00000    0.00000   -1.00000   -0.00023    0.00033

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  0.04 secs.
  Total Wall time:       0 mins.  0.25 secs.

  Calculation finished: Fri Sep 18 13:28:36 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.02 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:16:41 1998

  Run type: Single point energy
  Model: RHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   2
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Li Li1          0.0000000     3.4792904    -2.1635387

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  RHF direct SCF procedure requested

  Energy converged to -.16E-08 in   5 cycles

  E(HF)  =      -7.1870945 a.u.

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:      -2.76914   -0.19441   -0.12780   -0.12780   -0.12780

                        A          A          A          A          A
   1 Li  1 S        -0.99125   -0.19625    0.00000    0.00000    0.00000
   2 Li  1 S        -0.06263    0.37502    0.00000    0.00000    0.00000
   3 Li  1 PX        0.00000    0.00000   -0.02097    0.34164   -0.32317
   4 Li  1 PY        0.00000    0.00000    0.20175    0.29874    0.30273
   5 Li  1 PZ        0.00000    0.00000   -0.42480    0.12502    0.15973
   6 Li  1 S         0.02409    0.69199    0.00000    0.00000    0.00000
   7 Li  1 PX        0.00000    0.00000   -0.02886    0.47006   -0.44464
   8 Li  1 PY        0.00000    0.00000    0.27759    0.41103    0.41652
   9 Li  1 PZ        0.00000    0.00000   -0.58447    0.17201    0.21978

  MO:                   6          7          8          9

  Eigenvalues:       0.00341    0.00454    0.00454    0.00454

                        A          A          A          A
   1 Li  1 S         0.10652    0.00000    0.00000    0.00000
   2 Li  1 S        -1.57121    0.00000    0.00000    0.00000
   3 Li  1 PX        0.00000   -0.00592    0.00108   -1.14388
   4 Li  1 PY        0.00000   -1.06938   -0.40608    0.00515
   5 Li  1 PZ        0.00000   -0.40607    1.06939    0.00311
```

```
   6 Li  1 S         1.45013    0.00000    0.00000    0.00000
   7 Li  1 PX        0.00000    0.00545   -0.00099    1.05383
   8 Li  1 PY        0.00000    0.98520    0.37411   -0.00474
   9 Li  1 PZ        0.00000    0.37410   -0.98521   -0.00286

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  0.19 secs.
  Total Wall time:       0 mins.  0.43 secs.

  Calculation finished: Fri Sep 18 13:16:41 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.02 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:15:11 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   3
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Be Be1          0.0000000     2.8372787    -2.4822491

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.74E-05 in   5 cycles  <S**2> = 0.7500

  E(HF)  =     -14.1899719 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:      -5.13289   -0.65972   -0.22951   -0.22951   -0.22951

                        A          A          A          A          A
   1 Be  1 S        -0.99313   -0.21427    0.00000    0.00000    0.00000
   2 Be  1 S        -0.07384    0.42144    0.00000    0.00000    0.00000
   3 Be  1 PX        0.00000    0.00000   -0.30328    0.36155    0.15643
   4 Be  1 PY        0.00000    0.00000    0.27588    0.05401    0.41005
   5 Be  1 PZ        0.00000    0.00000    0.28120    0.33694   -0.23357
   6 Be  1 S         0.02790    0.64523    0.00000    0.00000    0.00000
   7 Be  1 PX        0.00000    0.00000   -0.38008    0.45310    0.19603
   8 Be  1 PY        0.00000    0.00000    0.34573    0.06768    0.51388
   9 Be  1 PZ        0.00000    0.00000    0.35241    0.42226   -0.29272

  MO:                   6          7          8          9

  Eigenvalues:       0.14532    0.14532    0.14532    0.24163

                        A          A          A          A
   1 Be  1 S         0.00000    0.00000    0.00000    0.01289
   2 Be  1 S         0.00000    0.00000    0.00000    1.60643
   3 Be  1 PX       -0.08913    0.41147   -1.05156    0.00000
   4 Be  1 PY        1.12685    0.10030   -0.05627    0.00000
   5 Be  1 PZ        0.07267   -1.05055   -0.41724    0.00000
```

```
  6 Be  1 S         0.00000    0.00000    0.00000   -1.54273
  7 Be  1 PX        0.08409   -0.38820    0.99209    0.00000
  8 Be  1 PY       -1.06312   -0.09462    0.05308    0.00000
  9 Be  1 PZ       -0.06856    0.99114    0.39364    0.00000

  Beta Spin Molecular Orbital Coefficients

  MO:                  1          2          3          4          5

  Eigenvalues:     -5.10095   -0.28891   -0.15966   -0.15966   -0.15966

                       A          A          A          A          A
  1 Be  1 S        -0.99275    0.21566    0.00000    0.00000    0.00000
  2 Be  1 S        -0.07638   -0.19512    0.00000    0.00000    0.00000
  3 Be  1 PX        0.00000    0.00000   -0.30144    0.20299   -0.16367
  4 Be  1 PY        0.00000    0.00000    0.25214    0.16312   -0.26206
  5 Be  1 PZ        0.00000    0.00000    0.06648    0.30174    0.25178
  6 Be  1 S         0.02840   -0.85241    0.00000    0.00000    0.00000
  7 Be  1 PX        0.00000    0.00000   -0.53853    0.36265   -0.29241
  8 Be  1 PY        0.00000    0.00000    0.45046    0.29142   -0.46818
  9 Be  1 PZ        0.00000    0.00000    0.11877    0.53906    0.44981

  MO:                  6          7          8          9

  Eigenvalues:      0.17446    0.17446    0.17446    0.30134

                       A          A          A          A
  1 Be  1 S         0.00000    0.00000    0.00000   -0.01820
  2 Be  1 S         0.00000    0.00000    0.00000    1.64917
  3 Be  1 PX       -0.03012    0.79177    0.86228    0.00000
  4 Be  1 PY       -1.05485   -0.39241    0.32348    0.00000
  5 Be  1 PZ       -0.50766    0.76841   -0.72330    0.00000
  6 Be  1 S         0.00000    0.00000    0.00000   -1.43865
  7 Be  1 PX        0.02601   -0.68391   -0.74482    0.00000
  8 Be  1 PY        0.91115    0.33896   -0.27941    0.00000
  9 Be  1 PZ        0.43851   -0.66373    0.62477    0.00000

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  0.20 secs.
  Total Wall time:       0 mins.  0.61 secs.

  Calculation finished: Fri Sep 18 13:15:12 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.03 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:11:58 1998

  Run type: Single point energy
  Model: RHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   4
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    B  B1           0.0000001    -2.6923087     4.3283113

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  RHF direct SCF procedure requested

  Energy converged to -.22E-07 in  10 cycles

  E(HF)  =     -24.0963762 a.u.

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:      -8.15612  -0.87230  -0.28034  -0.28034  -0.28034

                        A         A         A         A         A
   1 B   1 S        -0.98882  -0.23432   0.00000   0.00000   0.00000
   2 B   1 S        -0.07715   0.41074   0.00000   0.00000   0.00000
   3 B   1 PX        0.00000   0.00000  -0.45977  -0.16824  -0.14925
   4 B   1 PY        0.00000   0.00000   0.22428  -0.36824  -0.27581
   5 B   1 PZ        0.00000   0.00000   0.01672   0.31316  -0.40450
   6 B   1 S         0.02657   0.66500   0.00000   0.00000   0.00000
   7 B   1 PX        0.00000   0.00000  -0.55880  -0.20448  -0.18140
   8 B   1 PY        0.00000   0.00000   0.27259  -0.44755  -0.33522
   9 B   1 PZ        0.00000   0.00000   0.02032   0.38061  -0.49163

  MO:                   6         7         8         9

  Eigenvalues:       0.29715   0.29715   0.29715   0.42355

                        A         A         A         A
   1 B   1 S         0.00000   0.00000   0.00000  -0.06854
   2 B   1 S         0.00000   0.00000   0.00000   1.53209
   3 B   1 PX       -0.16903   0.08257   1.06734   0.00000
   4 B   1 PY       -0.27615   1.04063  -0.12423   0.00000
   5 B   1 PZ       -1.03430  -0.29133  -0.14126   0.00000
```

```
   6 B   1 S         0.00000    0.00000    0.00000   -1.43899
   7 B   1 PX        0.15978   -0.07805   -1.00895    0.00000
   8 B   1 PY        0.26104   -0.98370    0.11744    0.00000
   9 B   1 PZ        0.97771    0.27540    0.13353    0.00000

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  0.12 secs.
  Total Wall time:       0 mins.  0.19 secs.

  Calculation finished: Fri Sep 18 13:11:58 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.03 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:08:57 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   5
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  2

                     Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    C  C1          -0.0000001     2.1124265    -3.4283320

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.34E-05 in   5 cycles  <S**2> = 0.7505

  E(HF)  =     -37.0823086 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:     -11.87424   -1.21961   -0.90879   -0.37334   -0.37334

                        A          A          A          A          A
   1 C   1 S        -0.98635   -0.24743    0.00000    0.00000    0.00000
   2 C   1 S        -0.08410    0.36939    0.00000    0.00000    0.00000
   3 C   1 PX        0.00000    0.00000    0.67219    0.00000    0.00000
   4 C   1 PY        0.00000    0.00000    0.00000    0.33972   -0.39280
   5 C   1 PZ        0.00000    0.00000    0.00000   -0.39280   -0.33972
   6 C   1 S         0.02557    0.70854    0.00000    0.00000    0.00000
   7 C   1 PX        0.00000    0.00000    0.46576    0.00000    0.00000
   8 C   1 PY        0.00000    0.00000    0.00000    0.40750   -0.47117
   9 C   1 PZ        0.00000    0.00000    0.00000   -0.47117   -0.40750

  MO:                   6          7          8          9

  Eigenvalues:       0.45965    0.53655    0.53655    0.80933

                        A          A          A          A
   1 C   1 S         0.00000    0.00000    0.00000   -0.08375
   2 C   1 S         0.00000    0.00000    0.00000    1.50094
   3 C   1 PX        0.96781    0.00000    0.00000    0.00000
   4 C   1 PY        0.00000    1.01705   -0.29054    0.00000
   5 C   1 PZ        0.00000    0.29054    1.01705    0.00000
```

6 C	1 S	0.00000	0.00000	0.00000	-1.37238
7 C	1 PX	-1.08239	0.00000	0.00000	0.00000
8 C	1 PY	0.00000	-0.96175	0.27475	0.00000
9 C	1 PZ	0.00000	-0.27475	-0.96175	0.00000

Beta Spin Molecular Orbital Coefficients

MO:		1	2	3	4	5
Eigenvalues:		-11.84651	-1.08889	-0.34229	-0.34229	-0.28174
		A	A	A	A	A
1 C	1 S	0.98716	0.24267	0.00000	0.00000	0.00000
2 C	1 S	0.08094	-0.33523	0.00000	0.00000	0.00000
3 C	1 PX	0.00000	0.00000	0.00000	0.00000	-0.47455
4 C	1 PY	0.00000	0.00000	-0.35937	0.34942	0.00000
5 C	1 PZ	0.00000	0.00000	0.34942	0.35937	0.00000
6 C	1 S	-0.02566	-0.73963	0.00000	0.00000	0.00000
7 C	1 PX	0.00000	0.00000	0.00000	0.00000	-0.66430
8 C	1 PY	0.00000	0.00000	-0.45877	0.44607	0.00000
9 C	1 PZ	0.00000	0.00000	0.44607	0.45877	0.00000

MO:		6	7	8	9
Eigenvalues:		0.55439	0.55439	0.60648	0.85396
		A	A	A	A
1 C	1 S	0.00000	0.00000	0.00000	0.08794
2 C	1 S	0.00000	0.00000	0.00000	-1.50911
3 C	1 PX	0.00000	0.00000	1.07856	0.00000
4 C	1 PY	1.02690	0.28762	0.00000	0.00000
5 C	1 PZ	0.28762	-1.02690	0.00000	0.00000
6 C	1 S	0.00000	0.00000	0.00000	1.35587
7 C	1 PX	0.00000	0.00000	-0.97324	0.00000
8 C	1 PY	-0.95280	-0.26687	0.00000	0.00000
9 C	1 PZ	-0.26687	0.95280	0.00000	0.00000

** Archive file written to unit 12 **

Total Cpu time: 0 mins. 0.20 secs.
Total Wall time: 0 mins. 1.04 secs.

Calculation finished: Fri Sep 18 13:08:58 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

Total Cpu time: 0 mins. 0.03 secs.

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:21:28 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   6
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  3

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    N  N1          -0.0000001     1.3875744    -2.9318705

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.13E-05 in   5 cycles  <S**2> = 2.0013

  E(HF)  =     -53.5912731 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:     -16.27039   -1.61647   -1.11714   -1.11714   -0.47683

                        A          A          A          A          A
   1 N   1 S         0.98442    0.25577    0.00000    0.00000    0.00000
   2 N   1 S         0.09032   -0.34156    0.00000    0.00000    0.00000
   3 N   1 PX        0.00000    0.00000    0.00873    0.65291    0.00000
   4 N   1 PY        0.00000    0.00000   -0.65291    0.00873    0.00000
   5 N   1 PZ        0.00000    0.00000    0.00000    0.00000   -0.52584
   6 N   1 S        -0.02511   -0.73677    0.00000    0.00000    0.00000
   7 N   1 PX        0.00000    0.00000    0.00658    0.49197    0.00000
   8 N   1 PY        0.00000    0.00000   -0.49197    0.00658    0.00000
   9 N   1 PZ        0.00000    0.00000    0.00000    0.00000   -0.62148

  MO:                   6          7          8          9

  Eigenvalues:       0.74426    0.74426    0.83706    1.31309

                        A          A          A          A
   1 N   1 S         0.00000    0.00000    0.00000    0.09237
   2 N   1 S         0.00000    0.00000    0.00000   -1.48182
   3 N   1 PX        0.02118   -0.96750    0.00000    0.00000
   4 N   1 PY       -0.96750   -0.02118    0.00000    0.00000
   5 N   1 PZ        0.00000    0.00000    1.04229    0.00000
```

6 N	1 S	0.00000	0.00000	0.00000	1.32944
7 N	1 PX	-0.02317	1.05842	0.00000	0.00000
8 N	1 PY	1.05842	0.02317	0.00000	0.00000
9 N	1 PZ	0.00000	0.00000	-0.98825	0.00000

Beta Spin Molecular Orbital Coefficients

MO:		1	2	3	4	5
Eigenvalues:		-16.20107	-1.31274	-0.40250	-0.33019	-0.33019
		A	A	A	A	A
1 N	1 S	0.98593	0.24737	0.00000	0.00000	0.00000
2 N	1 S	0.08481	-0.28825	0.00000	0.00000	0.00000
3 N	1 PX	0.00000	0.00000	0.00000	-0.07542	-0.47046
4 N	1 PY	0.00000	0.00000	0.00000	-0.47046	0.07542
5 N	1 PZ	0.00000	0.00000	-0.49802	0.00000	0.00000
6 N	1 S	-0.02545	-0.78418	0.00000	0.00000	0.00000
7 N	1 PX	0.00000	0.00000	0.00000	-0.10559	-0.65866
8 N	1 PY	0.00000	0.00000	0.00000	-0.65866	0.10559
9 N	1 PZ	0.00000	0.00000	-0.64746	0.00000	0.00000

MO:		6	7	8	9
Eigenvalues:		0.87910	0.94177	0.94177	1.42219
		A	A	A	A
1 N	1 S	0.00000	0.00000	0.00000	-0.09886
2 N	1 S	0.00000	0.00000	0.00000	1.49343
3 N	1 PX	0.00000	0.18153	-1.05019	0.00000
4 N	1 PY	0.00000	-1.05019	-0.18153	0.00000
5 N	1 PZ	1.05586	0.00000	0.00000	0.00000
6 N	1 S	0.00000	0.00000	0.00000	-1.30204
7 N	1 PX	0.00000	-0.16319	0.94407	0.00000
8 N	1 PY	0.00000	0.94407	0.16319	0.00000
9 N	1 PZ	-0.97143	0.00000	0.00000	0.00000

** Archive file written to unit 12 **

Total Cpu time: 0 mins. 0.21 secs.
Total Wall time: 0 mins. 0.53 secs.

Calculation finished: Fri Sep 18 13:21:28 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

Total Cpu time: 0 mins. 0.03 secs.

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:26:48 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   7
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  4

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    O  O1           0.0000001     3.2307700    -2.0269174

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.68E-06 in   6 cycles  <S**2> = 3.7522

  E(HF)  =     -73.9589532 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:     -21.34682   -2.06462   -1.33770   -1.33770   -1.33770

                        A          A          A          A          A
   1 O   1 S         0.98195    0.26354    0.00000    0.00000    0.00000
   2 O   1 S         0.09344   -0.34269    0.00000    0.00000    0.00000
   3 O   1 PX        0.00000    0.00000    0.64660    0.03603   -0.02417
   4 O   1 PY        0.00000    0.00000    0.03704   -0.27039    0.58778
   5 O   1 PZ        0.00000    0.00000    0.02260   -0.58785   -0.27184
   6 O   1 S        -0.02394   -0.73968    0.00000    0.00000    0.00000
   7 O   1 PX        0.00000    0.00000    0.50299    0.02803   -0.01880
   8 O   1 PY        0.00000    0.00000    0.02881   -0.21034    0.45724
   9 O   1 PZ        0.00000    0.00000    0.01758   -0.45729   -0.21147

  MO:                   6          7          8          9

  Eigenvalues:       1.03892    1.03892    1.03892    1.78883

                        A          A          A          A
   1 O   1 S         0.00000    0.00000    0.00000   -0.11848
   2 O   1 S         0.00000    0.00000    0.00000    1.45334
   3 O   1 PX       -0.12036   -0.07768    0.94374    0.00000
   4 O   1 PY       -0.16658    0.93824    0.05598    0.00000
   5 O   1 PZ       -0.93217   -0.15764   -0.13186    0.00000
```

```
  6 O   1 S         0.00000    0.00000    0.00000   -1.29110
  7 O   1 PX        0.13086    0.08445   -1.02604    0.00000
  8 O   1 PY        0.18111   -1.02005   -0.06086    0.00000
  9 O   1 PZ        1.01345    0.17138    0.14336    0.00000

  Beta Spin Molecular Orbital Coefficients

  MO:                  1          2          3          4          5

  Eigenvalues:    -21.22072   -1.54709   -0.38390   -0.38390   -0.38390

                       A          A          A          A          A
  1 O   1 S        -0.98413   -0.25118    0.00000    0.00000    0.00000
  2 O   1 S        -0.08603    0.27493    0.00000    0.00000    0.00000
  3 O   1 PX        0.00000    0.00000    0.48261   -0.00654   -0.03203
  4 O   1 PY        0.00000    0.00000    0.02932   -0.12307    0.46688
  5 O   1 PZ        0.00000    0.00000   -0.01447   -0.46776   -0.12240
  6 O   1 S         0.02446    0.79910    0.00000    0.00000    0.00000
  7 O   1 PX        0.00000    0.00000    0.66508   -0.00902   -0.04414
  8 O   1 PY        0.00000    0.00000    0.04040   -0.16960    0.64340
  9 O   1 PZ        0.00000    0.00000   -0.01994   -0.64460   -0.16867

  MO:                  6          7          8          9

  Eigenvalues:      1.29382    1.29382    1.29382    1.98070

                       A          A          A          A
  1 O   1 S         0.00000    0.00000    0.00000   -0.12694
  2 O   1 S         0.00000    0.00000    0.00000    1.46812
  3 O   1 PX       -0.35059   -0.42902    0.88893    0.00000
  4 O   1 PY       -0.57328   -0.67941   -0.55400    0.00000
  5 O   1 PZ       -0.80350    0.67194    0.00740    0.00000
  6 O   1 S         0.00000    0.00000    0.00000   -1.25518
  7 O   1 PX        0.31519    0.38570   -0.79917    0.00000
  8 O   1 PY        0.51539    0.61081    0.49806    0.00000
  9 O   1 PZ        0.72237   -0.60409   -0.00666    0.00000

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  0.22 secs.
  Total Wall time:       0 mins.  0.48 secs.

  Calculation finished: Fri Sep 18 13:26:48 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.03 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:26:08 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   3
     1 S shells
     2 SP shells
  Number of basis functions:   9
  Number of electrons:   8
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  3

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    F  F1          -0.0000001     0.7455622    -1.5089561

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.39E-05 in   6 cycles  <S**2> = 2.0012

  E(HF)  =     -98.2787549 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:     -27.11498   -2.39135   -1.53936   -1.53936   -1.43221

                        A          A          A          A          A
   1 F   1 S         0.98114   -0.26491    0.00000    0.00000    0.00000
   2 F   1 S         0.09399    0.32173    0.00000    0.00000    0.00000
   3 F   1 PX        0.00000    0.00000    0.00000    0.00000    0.62610
   4 F   1 PY        0.00000    0.00000    0.61062   -0.18915    0.00000
   5 F   1 PZ        0.00000    0.00000    0.18915    0.61062    0.00000
   6 F   1 S        -0.02333    0.76062    0.00000    0.00000    0.00000
   7 F   1 PX        0.00000    0.00000    0.00000    0.00000    0.53179
   8 F   1 PY        0.00000    0.00000    0.49459   -0.15321    0.00000
   9 F   1 PZ        0.00000    0.00000    0.15321    0.49459    0.00000

  MO:                   6          7          8          9

  Eigenvalues:       1.41114    1.41114    1.48860    2.46622

                        A          A          A          A
   1 F   1 S         0.00000    0.00000    0.00000   -0.13102
   2 F   1 S         0.00000    0.00000    0.00000    1.44041
   3 F   1 PX        0.00000    0.00000   -0.95980    0.00000
   4 F   1 PY        0.51791   -0.79772    0.00000    0.00000
   5 F   1 PZ        0.79772    0.51791    0.00000    0.00000
```

6	F	1	S	0.00000	0.00000	0.00000	-1.25697
7	F	1	PX	0.00000	0.00000	1.01509	0.00000
8	F	1	PY	-0.55669	0.85745	0.00000	0.00000
9	F	1	PZ	-0.85745	-0.55669	0.00000	0.00000

Beta Spin Molecular Orbital Coefficients

MO:				1	2	3	4	5
Eigenvalues:				-27.01464	-2.00270	-1.31673	-0.50289	-0.50289
				A	A	A	A	A
1	F	1	S	0.98251	0.25722	0.00000	0.00000	0.00000
2	F	1	S	0.08947	-0.28240	0.00000	0.00000	0.00000
3	F	1	PX	0.00000	0.00000	0.60612	0.00000	0.00000
4	F	1	PY	0.00000	0.00000	0.00000	-0.17145	-0.47491
5	F	1	PZ	0.00000	0.00000	0.00000	-0.47491	0.17145
6	F	1	S	-0.02368	-0.79477	0.00000	0.00000	0.00000
7	F	1	PX	0.00000	0.00000	0.55266	0.00000	0.00000
8	F	1	PY	0.00000	0.00000	0.00000	-0.22110	-0.61243
9	F	1	PZ	0.00000	0.00000	0.00000	-0.61243	0.22110

MO:				6	7	8	9
Eigenvalues:				1.54457	1.67355	1.67355	2.61361
				A	A	A	A
1	F	1	S	0.00000	0.00000	0.00000	-0.13597
2	F	1	S	0.00000	0.00000	0.00000	1.44892
3	F	1	PX	-0.97254	0.00000	0.00000	0.00000
4	F	1	PY	0.00000	0.95192	0.39003	0.00000
5	F	1	PZ	0.00000	-0.39003	0.95192	0.00000
6	F	1	S	0.00000	0.00000	0.00000	-1.23565
7	F	1	PX	1.00388	0.00000	0.00000	0.00000
8	F	1	PY	0.00000	-0.87260	-0.35753	0.00000
9	F	1	PZ	0.00000	0.35753	-0.87260	0.00000

** Archive file written to unit 12 **

Total Cpu time: 0 mins. 0.21 secs.
Total Wall time: 0 mins. 0.53 secs.

Calculation finished: Fri Sep 18 13:26:08 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

Total Cpu time: 0 mins. 0.03 secs.

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:29:08 1998

  Run type: Single point energy
  Model: UHF/STO-3G
  Number of shells:   2
     1 S shells
     1 SP shells
  Number of basis functions:   5
  Number of electrons:   9
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Ne Ne1         -0.0000002     0.7041422    -3.4763319

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.28E-13 in   2 cycles  <S**2> = 0.7500

  E(HF)  =    -126.0614723 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:     -33.63976   -2.73372   -1.66966   -1.54820   -1.54820

                        A          A          A          A          A
   1 Ne  1 S         0.99517    0.26883    0.00000    0.00000    0.00000
   2 Ne  1 S         0.01917   -1.03066    0.00000    0.00000    0.00000
   3 Ne  1 PX        0.00000    0.00000    0.99994   -0.00131   -0.01051
   4 Ne  1 PY        0.00000    0.00000   -0.01051   -0.00298   -0.99994
   5 Ne  1 PZ        0.00000    0.00000   -0.00128   -0.99999    0.00299

  Beta Spin Molecular Orbital Coefficients

  MO:                   1          2          3          4          5

  Eigenvalues:     -33.60544   -2.51359   -1.48747   -1.48747   -0.54305

                        A          A          A          A          A
   1 Ne  1 S         0.99558    0.26732    0.00000    0.00000    0.00000
   2 Ne  1 S         0.01762   -1.03069    0.00000    0.00000    0.00000
   3 Ne  1 PX        0.00000    0.00000    0.01051   -0.00132   -0.99994
   4 Ne  1 PY        0.00000    0.00000    0.99993   -0.00455    0.01051
   5 Ne  1 PZ        0.00000    0.00000   -0.00457   -0.99999    0.00128

    ** Archive file written to unit 12 **
```

```
  Total Cpu time:        0 mins.  0.04 secs.
  Total Wall time:       0 mins.  0.17 secs.

  Calculation finished: Fri Sep 18 13:29:08 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.02 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:29:45 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  11
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Na Na1          0.0000000     2.7751482    -1.7280983

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.42E-10 in   9 cycles  <S**2> = 0.7500

  E(HF)  =    -160.8550531 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -40.21958   -2.77503   -1.48954   -1.48954   -1.48954

                        A         A         A         A         A
   1 Na  1 S         0.99048    0.26880    0.00000    0.00000    0.00000
   2 Na  1 S         0.03879   -1.02132    0.00000    0.00000    0.00000
   3 Na  1 PX        0.00000    0.00000    0.73707   -0.37166   -0.54904
   4 Na  1 PY        0.00000    0.00000   -0.23044   -0.91340    0.30895
   5 Na  1 PZ        0.00000    0.00000   -0.62168   -0.10208   -0.76548
   6 Na  1 S        -0.00653    0.04355    0.00000    0.00000    0.00000
   7 Na  1 PX        0.00000    0.00000    0.05430   -0.02738   -0.04045
   8 Na  1 PY        0.00000    0.00000   -0.01698   -0.06729    0.02276
   9 Na  1 PZ        0.00000    0.00000   -0.04580   -0.00752   -0.05639
  10 Na  1 S         0.00212   -0.00698    0.00000    0.00000    0.00000
  11 Na  1 PX        0.00000    0.00000   -0.02708    0.01365    0.02017
  12 Na  1 PY        0.00000    0.00000    0.00846    0.03355   -0.01135
  13 Na  1 PZ        0.00000    0.00000    0.02284    0.00375    0.02812
  14 Na  1 DXX       0.00018   -0.02949    0.00000    0.00000    0.00000
  15 Na  1 DYY       0.00018   -0.02949    0.00000    0.00000    0.00000
  16 Na  1 DZZ       0.00018   -0.02949    0.00000    0.00000    0.00000
  17 Na  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 Na  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 Na  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:		6	7	8	9	10
Eigenvalues:		-0.18051	0.02667	0.02667	0.02667	0.09474
		A	A	A	A	A
1	Na 1 S	-0.03845	0.00000	0.00000	0.00000	0.02587
2	Na 1 S	0.18995	0.00000	0.00000	0.00000	0.05538
3	Na 1 PX	0.00000	-0.06119	0.02581	0.00133	0.00000
4	Na 1 PY	0.00000	0.00857	0.02350	-0.06153	0.00000
5	Na 1 PZ	0.00000	-0.02438	-0.05651	-0.02498	0.00000
6	Na 1 S	-0.53593	0.00000	0.00000	0.00000	3.65534
7	Na 1 PX	0.00000	0.05079	-0.02142	-0.00110	0.00000
8	Na 1 PY	0.00000	-0.00712	-0.01950	0.05107	0.00000
9	Na 1 PZ	0.00000	0.02023	0.04691	0.02073	0.00000
10	Na 1 S	-0.51981	0.00000	0.00000	0.00000	-2.56304
11	Na 1 PX	0.00000	0.88198	-0.37196	-0.01916	0.00000
12	Na 1 PY	0.00000	-0.12356	-0.33868	0.88693	0.00000
13	Na 1 PZ	0.00000	0.35136	0.81459	0.36001	0.00000
14	Na 1 DXX	0.00483	0.00000	0.00000	0.00000	-0.55302
15	Na 1 DYY	0.00483	0.00000	0.00000	0.00000	-0.55302
16	Na 1 DZZ	0.00483	0.00000	0.00000	0.00000	-0.55302
17	Na 1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Na 1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Na 1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.15414	0.15414	0.15414	0.46351	0.46351
		A	A	A	A	A
1	Na 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2	Na 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3	Na 1 PX	0.06996	-0.17376	-0.00163	0.00000	0.00000
4	Na 1 PY	-0.13866	-0.05477	-0.11341	0.00000	0.00000
5	Na 1 PZ	-0.10472	-0.04357	0.14908	0.00000	0.00000
6	Na 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7	Na 1 PX	-0.59702	1.48274	0.01395	0.00000	0.00000
8	Na 1 PY	1.18327	0.46734	0.96778	0.00000	0.00000
9	Na 1 PZ	0.89363	0.37179	-1.27214	0.00000	0.00000
10	Na 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11	Na 1 PX	0.47423	-1.17778	-0.01108	0.00000	0.00000
12	Na 1 PY	-0.93991	-0.37122	-0.76874	0.00000	0.00000
13	Na 1 PZ	-0.70984	-0.29532	1.01050	0.00000	0.00000
14	Na 1 DXX	0.00000	0.00000	0.00000	-0.00441	-0.01270
15	Na 1 DYY	0.00000	0.00000	0.00000	0.00248	0.28290
16	Na 1 DZZ	0.00000	0.00000	0.00000	0.00192	-0.27020
17	Na 1 DXY	0.00000	0.00000	0.00000	-0.54203	0.33517
18	Na 1 DXZ	0.00000	0.00000	0.00000	0.22479	-0.77047
19	Na 1 DYZ	0.00000	0.00000	0.00000	0.80973	0.43806

MO:		16	17	18	19
Eigenvalues:		0.46351	0.46351	0.46351	0.51590
		A	A	A	A
1	Na 1 S	0.00000	0.00000	0.00000	0.00255
2	Na 1 S	0.00000	0.00000	0.00000	-0.11950
3	Na 1 PX	0.00000	0.00000	0.00000	0.00000
4	Na 1 PY	0.00000	0.00000	0.00000	0.00000
5	Na 1 PZ	0.00000	0.00000	0.00000	0.00000

6	Na	1	S	0.00000	0.00000	0.00000	-6.51987
7	Na	1	PX	0.00000	0.00000	0.00000	0.00000
8	Na	1	PY	0.00000	0.00000	0.00000	0.00000
9	Na	1	PZ	0.00000	0.00000	0.00000	0.00000
10	Na	1	S	0.00000	0.00000	0.00000	2.00920
11	Na	1	PX	0.00000	0.00000	0.00000	0.00000
12	Na	1	PY	0.00000	0.00000	0.00000	0.00000
13	Na	1	PZ	0.00000	0.00000	0.00000	0.00000
14	Na	1	DXX	-0.56012	-0.82821	0.01240	2.26914
15	Na	1	DYY	0.26230	0.43415	0.81405	2.26914
16	Na	1	DZZ	0.29782	0.39406	-0.82644	2.26914
17	Na	1	DXY	0.63244	-0.43131	-0.08858	0.00000
18	Na	1	DXZ	0.44466	-0.28597	0.27631	0.00000
19	Na	1	DYZ	0.29688	-0.21385	-0.13632	0.00000

Beta Spin Molecular Orbital Coefficients

MO:				1	2	3	4	5
Eigenvalues:				-40.21718	-2.76862	-1.48745	-1.48745	-1.48745
				A	A	A	A	A
1	Na	1	S	0.99047	0.26880	0.00000	0.00000	0.00000
2	Na	1	S	0.03882	-1.02122	0.00000	0.00000	0.00000
3	Na	1	PX	0.00000	0.00000	-0.81918	0.08660	-0.55278
4	Na	1	PY	0.00000	0.00000	-0.10377	0.93955	0.30098
5	Na	1	PZ	0.00000	0.00000	0.54982	0.30637	-0.76679
6	Na	1	S	-0.00653	0.04309	0.00000	0.00000	0.00000
7	Na	1	PX	0.00000	0.00000	-0.05672	0.00600	-0.03828
8	Na	1	PY	0.00000	0.00000	-0.00719	0.06506	0.02084
9	Na	1	PZ	0.00000	0.00000	0.03807	0.02121	-0.05309
10	Na	1	S	0.00212	-0.00674	0.00000	0.00000	0.00000
11	Na	1	PX	0.00000	0.00000	0.02908	-0.00307	0.01963
12	Na	1	PY	0.00000	0.00000	0.00368	-0.03336	-0.01069
13	Na	1	PZ	0.00000	0.00000	-0.01952	-0.01088	0.02722
14	Na	1	DXX	0.00018	-0.02965	0.00000	0.00000	0.00000
15	Na	1	DYY	0.00018	-0.02965	0.00000	0.00000	0.00000
16	Na	1	DZZ	0.00018	-0.02965	0.00000	0.00000	0.00000
17	Na	1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Na	1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Na	1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:				6	7	8	9	10
Eigenvalues:				0.01678	0.04946	0.04946	0.04946	0.12770
				A	A	A	A	A
1	Na	1	S	0.02600	0.00000	0.00000	0.00000	-0.03833
2	Na	1	S	-0.19427	0.00000	0.00000	0.00000	0.01454
3	Na	1	PX	0.00000	-0.02269	-0.01427	0.01920	0.00000
4	Na	1	PY	0.00000	0.00305	-0.02797	-0.01719	0.00000
5	Na	1	PZ	0.00000	-0.02373	0.01005	-0.02057	0.00000
6	Na	1	S	-0.71251	0.00000	0.00000	0.00000	-3.88399
7	Na	1	PX	0.00000	-0.14320	-0.09009	0.12118	0.00000
8	Na	1	PY	0.00000	0.01924	-0.17654	-0.10850	0.00000
9	Na	1	PZ	0.00000	-0.14977	0.06345	-0.12981	0.00000
10	Na	1	S	1.39208	0.00000	0.00000	0.00000	2.27291
11	Na	1	PX	0.00000	0.79336	0.49909	-0.67137	0.00000
12	Na	1	PY	0.00000	-0.10662	0.97805	0.60108	0.00000
13	Na	1	PZ	0.00000	0.82973	-0.35153	0.71917	0.00000
14	Na	1	DXX	0.14733	0.00000	0.00000	0.00000	0.61753

```
15 Na  1 DYY       0.14733    0.00000    0.00000    0.00000    0.61753
16 Na  1 DZZ       0.14733    0.00000    0.00000    0.00000    0.61753
17 Na  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
18 Na  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
19 Na  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000

MO:                  11         12         13         14         15

Eigenvalues:       0.18514    0.18514    0.18514    0.48671    0.48671

                      A          A          A          A          A
 1 Na  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
 2 Na  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
 3 Na  1 PX        0.12622    0.07687   -0.12373    0.00000    0.00000
 4 Na  1 PY       -0.07955    0.17352    0.02665    0.00000    0.00000
 5 Na  1 PZ       -0.12202   -0.03362   -0.14536    0.00000    0.00000
 6 Na  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
 7 Na  1 PX       -1.03864   -0.63256    1.01813    0.00000    0.00000
 8 Na  1 PY        0.65465   -1.42788   -0.21929    0.00000    0.00000
 9 Na  1 PZ        1.00407    0.27664    1.19616    0.00000    0.00000
10 Na  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
11 Na  1 PX        0.71726    0.43683   -0.70310    0.00000    0.00000
12 Na  1 PY       -0.45209    0.98607    0.15144    0.00000    0.00000
13 Na  1 PZ       -0.69339   -0.19104   -0.82605    0.00000    0.00000
14 Na  1 DXX       0.00000    0.00000    0.00000   -0.24862   -0.86538
15 Na  1 DYY       0.00000    0.00000    0.00000   -0.66771    0.64126
16 Na  1 DZZ       0.00000    0.00000    0.00000    0.91633    0.22413
17 Na  1 DXY       0.00000    0.00000    0.00000    0.10025   -0.35173
18 Na  1 DXZ       0.00000    0.00000    0.00000   -0.27005   -0.22170
19 Na  1 DYZ       0.00000    0.00000    0.00000    0.13717   -0.14228

MO:                  16         17         18         19

Eigenvalues:       0.48671    0.48671    0.48671    0.53051

                      A          A          A          A
 1 Na  1 S         0.00000    0.00000    0.00000    0.00497
 2 Na  1 S         0.00000    0.00000    0.00000   -0.12519
 3 Na  1 PX        0.00000    0.00000    0.00000    0.00000
 4 Na  1 PY        0.00000    0.00000    0.00000    0.00000
 5 Na  1 PZ        0.00000    0.00000    0.00000    0.00000
 6 Na  1 S         0.00000    0.00000    0.00000   -6.36902
 7 Na  1 PX        0.00000    0.00000    0.00000    0.00000
 8 Na  1 PY        0.00000    0.00000    0.00000    0.00000
 9 Na  1 PZ        0.00000    0.00000    0.00000    0.00000
10 Na  1 S         0.00000    0.00000    0.00000    1.94223
11 Na  1 PX        0.00000    0.00000    0.00000    0.00000
12 Na  1 PY        0.00000    0.00000    0.00000    0.00000
13 Na  1 PZ        0.00000    0.00000    0.00000    0.00000
14 Na  1 DXX      -0.42544   -0.09029    0.01190    2.24763
15 Na  1 DYY       0.30738   -0.21982   -0.01236    2.24763
16 Na  1 DZZ       0.11806    0.31011    0.00046    2.24763
17 Na  1 DXY       0.70838   -0.31092   -0.51746    0.00000
18 Na  1 DXZ       0.44842    0.78714    0.23928    0.00000
19 Na  1 DYZ       0.32276   -0.42660    0.82145    0.00000

  ** Archive file written to unit 12 **

Total Cpu time:        0 mins.  1.48 secs.
Total Wall time:       0 mins.  1.94 secs.
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  Calculation finished: Fri Sep 18 13:29:47 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
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```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:31:12 1998

  Run type: Single point energy
  Model: RHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  12
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Mg Mg1          0.0000001     1.2011839     2.6260351

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  RHF direct SCF procedure requested

  Energy converged to -.43E-07 in   6 cycles

  E(HF)  =    -198.4852920 a.u.

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -48.69517   -3.73941   -2.24856   -2.24856   -2.24856

                        A         A         A         A         A
   1 Mg  1 S        -0.98872   -0.27476    0.00000    0.00000    0.00000
   2 Mg  1 S        -0.04680    1.00013    0.00000    0.00000    0.00000
   3 Mg  1 PX        0.00000    0.00000   -0.42934    0.60632   -0.64105
   4 Mg  1 PY        0.00000    0.00000    0.07308   -0.68602   -0.69780
   5 Mg  1 PZ        0.00000    0.00000    0.87933    0.35305   -0.25500
   6 Mg  1 S         0.03294    0.14888    0.00000    0.00000    0.00000
   7 Mg  1 PX        0.00000    0.00000   -0.03875    0.05473   -0.05786
   8 Mg  1 PY        0.00000    0.00000    0.00660   -0.06192   -0.06298
   9 Mg  1 PZ        0.00000    0.00000    0.07937    0.03187   -0.02302
  10 Mg  1 S         0.01236    0.01557    0.00000    0.00000    0.00000
  11 Mg  1 PX        0.00000    0.00000    0.01443   -0.02038    0.02155
  12 Mg  1 PY        0.00000    0.00000   -0.00246    0.02306    0.02346
  13 Mg  1 PZ        0.00000    0.00000   -0.02956   -0.01187    0.00857
  14 Mg  1 DXX      -0.01731   -0.05254    0.00000    0.00000    0.00000
  15 Mg  1 DYY      -0.01731   -0.05254    0.00000    0.00000    0.00000
  16 Mg  1 DZZ      -0.01731   -0.05254    0.00000    0.00000    0.00000
  17 Mg  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 Mg  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 Mg  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:		6	7	8	9	10
Eigenvalues:		-0.25181	0.04857	0.04857	0.04857	0.23468
		A	A	A	A	A
1	Mg 1 S	-0.04935	0.00000	0.00000	0.00000	-0.03149
2	Mg 1 S	0.26123	0.00000	0.00000	0.00000	-0.01213
3	Mg 1 PX	0.00000	-0.10266	-0.00443	-0.02021	0.00000
4	Mg 1 PY	0.00000	0.02051	-0.00833	-0.10236	0.00000
5	Mg 1 PZ	0.00000	-0.00272	0.10430	-0.00904	0.00000
6	Mg 1 S	-0.32625	0.00000	0.00000	0.00000	-1.41402
7	Mg 1 PX	0.00000	0.10395	0.00449	0.02046	0.00000
8	Mg 1 PY	0.00000	-0.02077	0.00844	0.10365	0.00000
9	Mg 1 PZ	0.00000	0.00276	-0.10561	0.00915	0.00000
10	Mg 1 S	-0.67166	0.00000	0.00000	0.00000	1.92551
11	Mg 1 PX	0.00000	0.90828	0.03922	0.17879	0.00000
12	Mg 1 PY	0.00000	-0.18145	0.07373	0.90561	0.00000
13	Mg 1 PZ	0.00000	0.02410	-0.92277	0.07996	0.00000
14	Mg 1 DXX	-0.02856	0.00000	0.00000	0.00000	-0.26531
15	Mg 1 DYY	-0.02856	0.00000	0.00000	0.00000	-0.26531
16	Mg 1 DZZ	-0.02856	0.00000	0.00000	0.00000	-0.26531
17	Mg 1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Mg 1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Mg 1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.32183	0.32183	0.32183	0.43321	0.43321
		A	A	A	A	A
1	Mg 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2	Mg 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3	Mg 1 PX	-0.05263	0.15593	-0.24190	0.00000	0.00000
4	Mg 1 PY	-0.28503	-0.06231	0.02185	0.00000	0.00000
5	Mg 1 PZ	-0.03987	0.23959	0.16312	0.00000	0.00000
6	Mg 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7	Mg 1 PX	0.25259	-0.74833	1.16088	0.00000	0.00000
8	Mg 1 PY	1.36786	0.29901	-0.10488	0.00000	0.00000
9	Mg 1 PZ	0.19132	-1.14980	-0.78282	0.00000	0.00000
10	Mg 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11	Mg 1 PX	-0.18456	0.54680	-0.84824	0.00000	0.00000
12	Mg 1 PY	-0.99948	-0.21848	0.07663	0.00000	0.00000
13	Mg 1 PZ	-0.13980	0.84014	0.57200	0.00000	0.00000
14	Mg 1 DXX	0.00000	0.00000	0.00000	-0.51834	-0.72617
15	Mg 1 DYY	0.00000	0.00000	0.00000	0.99629	-0.02104
16	Mg 1 DZZ	0.00000	0.00000	0.00000	-0.47795	0.74722
17	Mg 1 DXY	0.00000	0.00000	0.00000	-0.08279	-0.00921
18	Mg 1 DXZ	0.00000	0.00000	0.00000	0.00113	-0.43943
19	Mg 1 DYZ	0.00000	0.00000	0.00000	0.00301	0.28765

MO:		16	17	18	19
Eigenvalues:		0.43321	0.43321	0.43321	0.93164
		A	A	A	A
1	Mg 1 S	0.00000	0.00000	0.00000	0.09696
2	Mg 1 S	0.00000	0.00000	0.00000	-0.58075
3	Mg 1 PX	0.00000	0.00000	0.00000	0.00000
4	Mg 1 PY	0.00000	0.00000	0.00000	0.00000
5	Mg 1 PZ	0.00000	0.00000	0.00000	0.00000

```
   6 Mg   1 S          0.00000    0.00000    0.00000    2.77408
   7 Mg   1 PX         0.00000    0.00000    0.00000    0.00000
   8 Mg   1 PY         0.00000    0.00000    0.00000    0.00000
   9 Mg   1 PZ         0.00000    0.00000    0.00000    0.00000
  10 Mg   1 S          0.00000    0.00000    0.00000    1.31147
  11 Mg   1 PX         0.00000    0.00000    0.00000    0.00000
  12 Mg   1 PY         0.00000    0.00000    0.00000    0.00000
  13 Mg   1 PZ         0.00000    0.00000    0.00000    0.00000
  14 Mg   1 DXX        0.44994   -0.02477    0.03059   -1.76273
  15 Mg   1 DYY        0.00690    0.08313    0.00273   -1.76273
  16 Mg   1 DZZ       -0.45685   -0.05836   -0.03333   -1.76273
  17 Mg   1 DXY       -0.05972    0.99287    0.06081    0.00000
  18 Mg   1 DXZ       -0.74586   -0.07912    0.49430    0.00000
  19 Mg   1 DYZ        0.40741   -0.02564    0.86637    0.00000

    ** Archive file written to unit 12 **

  Total Cpu time:         0 mins.  1.22 secs.
  Total Wall time:        0 mins.  2.58 secs.

  Calculation finished: Fri Sep 18 13:31:14 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:32:37 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  13
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Al Al1         -0.0000001     0.0000000    -1.1017752

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.22E-05 in   6 cycles  <S**2> = 0.7570

  E(HF)  =    -240.5869385 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -58.12595   -4.88329   -3.19202   -3.18588   -3.18588

                        A         A         A         A         A
   1 Al  1 S         0.98701    0.28060    0.00000    0.00000    0.00000
   2 Al  1 S         0.05420   -0.98900    0.00000    0.00000    0.00000
   3 Al  1 PX        0.00000    0.00000    0.98029    0.00000    0.00000
   4 Al  1 PY        0.00000    0.00000    0.00000   -0.83622   -0.50979
   5 Al  1 PZ        0.00000    0.00000    0.00000    0.50979   -0.83622
   6 Al  1 S        -0.09460   -0.27067    0.00000    0.00000    0.00000
   7 Al  1 PX        0.00000    0.00000    0.08006    0.00000    0.00000
   8 Al  1 PY        0.00000    0.00000    0.00000   -0.07136   -0.04350
   9 Al  1 PZ        0.00000    0.00000    0.00000    0.04350   -0.07136
  10 Al  1 S        -0.00004    0.02459    0.00000    0.00000    0.00000
  11 Al  1 PX        0.00000    0.00000   -0.02733    0.00000    0.00000
  12 Al  1 PY        0.00000    0.00000    0.00000    0.02467    0.01504
  13 Al  1 PZ        0.00000    0.00000    0.00000   -0.01504    0.02467
  14 Al  1 DXX       0.03867    0.08463    0.00000    0.00000    0.00000
  15 Al  1 DYY       0.03869    0.08464    0.00000    0.00000    0.00000
  16 Al  1 DZZ       0.03869    0.08464    0.00000    0.00000    0.00000
  17 Al  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 Al  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 Al  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:		6	7	8	9	10
Eigenvalues:		-0.42114	-0.21561	0.02650	0.02650	0.29237
		A	A	A	A	A
1	Al 1 S	0.05945	0.00000	0.00000	0.00000	-0.05405
2	Al 1 S	-0.29997	0.00000	0.00000	0.00000	0.10240
3	Al 1 PX	0.00000	0.19317	0.00000	0.00000	0.00000
4	Al 1 PY	0.00000	0.00000	0.14625	-0.00037	0.00000
5	Al 1 PZ	0.00000	0.00000	0.00037	0.14625	0.00000
6	Al 1 S	0.38094	0.00000	0.00000	0.00000	-1.52603
7	Al 1 PX	0.00000	-0.46700	0.00000	0.00000	0.00000
8	Al 1 PY	0.00000	0.00000	-0.25638	0.00064	0.00000
9	Al 1 PZ	0.00000	0.00000	-0.00064	-0.25638	0.00000
10	Al 1 S	0.60856	0.00000	0.00000	0.00000	1.67377
11	Al 1 PX	0.00000	-0.63792	0.00000	0.00000	0.00000
12	Al 1 PY	0.00000	0.00000	-0.81664	0.00205	0.00000
13	Al 1 PZ	0.00000	0.00000	-0.00205	-0.81664	0.00000
14	Al 1 DXX	0.08058	0.00000	0.00000	0.00000	-0.08793
15	Al 1 DYY	0.01743	0.00000	0.00000	0.00000	-0.09575
16	Al 1 DZZ	0.01743	0.00000	0.00000	0.00000	-0.09575
17	Al 1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Al 1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Al 1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.34777	0.37602	0.37602	0.63859	0.64241
		A	A	A	A	A
1	Al 1 S	0.00000	0.00000	0.00000	0.00232	0.00000
2	Al 1 S	0.00000	0.00000	0.00000	-0.01278	0.00000
3	Al 1 PX	0.29164	0.00000	0.00000	0.00000	0.00000
4	Al 1 PY	0.00000	-0.27138	0.17073	0.00000	0.00000
5	Al 1 PZ	0.00000	0.17073	0.27138	0.00000	0.00000
6	Al 1 S	0.00000	0.00000	0.00000	0.01343	0.00000
7	Al 1 PX	-1.30664	0.00000	0.00000	0.00000	0.00000
8	Al 1 PY	0.00000	1.15410	-0.72605	0.00000	0.00000
9	Al 1 PZ	0.00000	-0.72605	-1.15410	0.00000	0.00000
10	Al 1 S	0.00000	0.00000	0.00000	0.03463	0.00000
11	Al 1 PX	1.19063	0.00000	0.00000	0.00000	0.00000
12	Al 1 PY	0.00000	-0.91067	0.57291	0.00000	0.00000
13	Al 1 PZ	0.00000	0.57291	0.91067	0.00000	0.00000
14	Al 1 DXX	0.00000	0.00000	0.00000	-1.00041	0.00000
15	Al 1 DYY	0.00000	0.00000	0.00000	0.49824	0.00000
16	Al 1 DZZ	0.00000	0.00000	0.00000	0.49824	0.00000
17	Al 1 DXY	0.00000	0.00000	0.00000	0.00000	-0.49607
18	Al 1 DXZ	0.00000	0.00000	0.00000	0.00000	-0.86828
19	Al 1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		16	17	18	19
Eigenvalues:		0.64241	0.65754	0.65754	1.94575
		A	A	A	A
1	Al 1 S	0.00000	0.00000	0.00000	0.13266
2	Al 1 S	0.00000	0.00000	0.00000	-0.79335
3	Al 1 PX	0.00000	0.00000	0.00000	0.00000
4	Al 1 PY	0.00000	0.00000	0.00000	0.00000
5	Al 1 PZ	0.00000	0.00000	0.00000	0.00000

6	Al	1	S	0.00000	0.00000	0.00000	6.20820
7	Al	1	PX	0.00000	0.00000	0.00000	0.00000
8	Al	1	PY	0.00000	0.00000	0.00000	0.00000
9	Al	1	PZ	0.00000	0.00000	0.00000	0.00000
10	Al	1	S	0.00000	0.00000	0.00000	0.28963
11	Al	1	PX	0.00000	0.00000	0.00000	0.00000
12	Al	1	PY	0.00000	0.00000	0.00000	0.00000
13	Al	1	PZ	0.00000	0.00000	0.00000	0.00000
14	Al	1	DXX	0.00000	0.00000	0.00000	-2.84103
15	Al	1	DYY	0.00000	-0.79388	0.34607	-2.84232
16	Al	1	DZZ	0.00000	0.79388	-0.34607	-2.84232
17	Al	1	DXY	0.86828	0.00000	0.00000	0.00000
18	Al	1	DXZ	-0.49607	0.00000	0.00000	0.00000
19	Al	1	DYZ	0.00000	-0.39960	-0.91669	0.00000

Beta Spin Molecular Orbital Coefficients

MO:				1	2	3	4	5
Eigenvalues:				-58.12339	-4.88012	-3.18463	-3.18463	-3.17521
				A	A	A	A	A
1	Al	1	S	0.98703	0.28058	0.00000	0.00000	0.00000
2	Al	1	S	0.05414	-0.98904	0.00000	0.00000	0.00000
3	Al	1	PX	0.00000	0.00000	0.00000	0.00000	0.98001
4	Al	1	PY	0.00000	0.00000	0.86237	-0.46422	0.00000
5	Al	1	PZ	0.00000	0.00000	-0.46422	-0.86237	0.00000
6	Al	1	S	-0.09447	-0.27159	0.00000	0.00000	0.00000
7	Al	1	PX	0.00000	0.00000	0.00000	0.00000	0.08129
8	Al	1	PY	0.00000	0.00000	0.07359	-0.03961	0.00000
9	Al	1	PZ	0.00000	0.00000	-0.03961	-0.07359	0.00000
10	Al	1	S	-0.00004	0.02479	0.00000	0.00000	0.00000
11	Al	1	PX	0.00000	0.00000	0.00000	0.00000	-0.02840
12	Al	1	PY	0.00000	0.00000	-0.02555	0.01375	0.00000
13	Al	1	PZ	0.00000	0.00000	0.01375	0.02555	0.00000
14	Al	1	DXX	0.03863	0.08595	0.00000	0.00000	0.00000
15	Al	1	DYY	0.03863	0.08491	0.00000	0.00000	0.00000
16	Al	1	DZZ	0.03863	0.08491	0.00000	0.00000	0.00000
17	Al	1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Al	1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Al	1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:				6	7	8	9	10
Eigenvalues:				-0.35868	0.03863	0.03863	0.07429	0.30851
				A	A	A	A	A
1	Al	1	S	0.06051	0.00000	0.00000	0.00000	-0.05325
2	Al	1	S	-0.30472	0.00000	0.00000	0.00000	0.09841
3	Al	1	PX	0.00000	0.00000	0.00000	0.13230	0.00000
4	Al	1	PY	0.00000	0.14452	0.01116	0.00000	0.00000
5	Al	1	PZ	0.00000	-0.01116	0.14452	0.00000	0.00000
6	Al	1	S	0.43013	0.00000	0.00000	0.00000	-1.51682
7	Al	1	PX	0.00000	0.00000	0.00000	-0.20257	0.00000
8	Al	1	PY	0.00000	-0.25066	-0.01935	0.00000	0.00000
9	Al	1	PZ	0.00000	0.01935	-0.25066	0.00000	0.00000
10	Al	1	S	0.59398	0.00000	0.00000	0.00000	1.67983
11	Al	1	PX	0.00000	0.00000	0.00000	-0.85836	0.00000
12	Al	1	PY	0.00000	-0.81814	-0.06316	0.00000	0.00000
13	Al	1	PZ	0.00000	0.06316	-0.81814	0.00000	0.00000
14	Al	1	DXX	-0.01709	0.00000	0.00000	0.00000	-0.06259

```
15 Al  1 DYY       0.04398    0.00000    0.00000    0.00000   -0.11051
16 Al  1 DZZ       0.04398    0.00000    0.00000    0.00000   -0.11051
17 Al  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
18 Al  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
19 Al  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000

MO:                  11         12         13         14         15

Eigenvalues:       0.37992    0.37992    0.41323    0.65955    0.65955

                      A          A          A          A          A
 1 Al  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
 2 Al  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
 3 Al  1 PX        0.00000    0.00000    0.32467    0.00000    0.00000
 4 Al  1 PY        0.23473    0.21920    0.00000    0.00000    0.00000
 5 Al  1 PZ       -0.21920    0.23473    0.00000    0.00000    0.00000
 6 Al  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
 7 Al  1 PX        0.00000    0.00000   -1.37265    0.00000    0.00000
 8 Al  1 PY       -0.99720   -0.93124    0.00000    0.00000    0.00000
 9 Al  1 PZ        0.93124   -0.99720    0.00000    0.00000    0.00000
10 Al  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
11 Al  1 PX        0.00000    0.00000    1.04293    0.00000    0.00000
12 Al  1 PY        0.78415    0.73228    0.00000    0.00000    0.00000
13 Al  1 PZ       -0.73228    0.78415    0.00000    0.00000    0.00000
14 Al  1 DXX       0.00000    0.00000    0.00000    0.00000    0.00000
15 Al  1 DYY       0.00000    0.00000    0.00000    0.76902   -0.39827
16 Al  1 DZZ       0.00000    0.00000    0.00000   -0.76902    0.39827
17 Al  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
18 Al  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
19 Al  1 DYZ       0.00000    0.00000    0.00000   -0.45988   -0.88798

MO:                  16         17         18         19

Eigenvalues:       0.69050    0.69050    0.70232    1.95491

                      A          A          A          A
 1 Al  1 S         0.00000    0.00000    0.00478   -0.13238
 2 Al  1 S         0.00000    0.00000   -0.01966    0.79185
 3 Al  1 PX        0.00000    0.00000    0.00000    0.00000
 4 Al  1 PY        0.00000    0.00000    0.00000    0.00000
 5 Al  1 PZ        0.00000    0.00000    0.00000    0.00000
 6 Al  1 S         0.00000    0.00000    0.10367   -6.20635
 7 Al  1 PX        0.00000    0.00000    0.00000    0.00000
 8 Al  1 PY        0.00000    0.00000    0.00000    0.00000
 9 Al  1 PZ        0.00000    0.00000    0.00000    0.00000
10 Al  1 S         0.00000    0.00000   -0.02782   -0.28545
11 Al  1 PX        0.00000    0.00000    0.00000    0.00000
12 Al  1 PY        0.00000    0.00000    0.00000    0.00000
13 Al  1 PZ        0.00000    0.00000    0.00000    0.00000
14 Al  1 DXX       0.00000    0.00000    0.98543    2.84798
15 Al  1 DYY       0.00000    0.00000   -0.51253    2.83895
16 Al  1 DZZ       0.00000    0.00000   -0.51253    2.83895
17 Al  1 DXY      -0.25611    0.96665    0.00000    0.00000
18 Al  1 DXZ       0.96665    0.25611    0.00000    0.00000
19 Al  1 DYZ       0.00000    0.00000    0.00000    0.00000

  ** Archive file written to unit 12 **

Total Cpu time:        0 mins.  1.39 secs.
Total Wall time:       0 mins.  2.53 secs.
```

```
  Calculation finished: Fri Sep 18 13:32:39 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:33:54 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  14
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  3

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Si Si1          0.0000000     2.3195269    -0.9577253

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.36E-05 in   5 cycles  <S**2> = 2.0061

  E(HF)  =    -287.3944670 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -68.39310   -6.13597   -4.23872   -4.23872   -4.22925

                        A         A         A         A         A
   1 Si  1 S        -0.98614   -0.28623    0.00000    0.00000    0.00000
   2 Si  1 S        -0.06094    0.97114    0.00000    0.00000    0.00000
   3 Si  1 PX        0.00000    0.00000   -0.95189    0.21648    0.00000
   4 Si  1 PY        0.00000    0.00000    0.21648    0.95189    0.00000
   5 Si  1 PZ        0.00000    0.00000    0.00000    0.00000    0.97494
   6 Si  1 S         0.10315    0.30858    0.00000    0.00000    0.00000
   7 Si  1 PX        0.00000    0.00000   -0.08110    0.01844    0.00000
   8 Si  1 PY        0.00000    0.00000    0.01844    0.08110    0.00000
   9 Si  1 PZ        0.00000    0.00000    0.00000    0.00000    0.08729
  10 Si  1 S         0.00352   -0.01805    0.00000    0.00000    0.00000
  11 Si  1 PX        0.00000    0.00000    0.02451   -0.00557    0.00000
  12 Si  1 PY        0.00000    0.00000   -0.00557   -0.02451    0.00000
  13 Si  1 PZ        0.00000    0.00000    0.00000    0.00000   -0.02681
  14 Si  1 DXX      -0.04278   -0.09677    0.00000    0.00000    0.00000
  15 Si  1 DYY      -0.04278   -0.09677    0.00000    0.00000    0.00000
  16 Si  1 DZZ      -0.04280   -0.09686    0.00000    0.00000    0.00000
  17 Si  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 Si  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 Si  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:		6	7	8	9	10
Eigenvalues:		-0.61460	-0.29909	-0.29909	-0.00022	0.40899
		A	A	A	A	A
1 Si	1 S	-0.06652	0.00000	0.00000	0.00000	0.06054
2 Si	1 S	0.34464	0.00000	0.00000	0.00000	-0.14932
3 Si	1 PX	0.00000	-0.22661	0.02424	0.00000	0.00000
4 Si	1 PY	0.00000	-0.02424	-0.22661	0.00000	0.00000
5 Si	1 PZ	0.00000	0.00000	0.00000	0.18492	0.00000
6 Si	1 S	-0.35128	0.00000	0.00000	0.00000	1.50654
7 Si	1 PX	0.00000	0.48842	-0.05225	0.00000	0.00000
8 Si	1 PY	0.00000	0.05225	0.48842	0.00000	0.00000
9 Si	1 PZ	0.00000	0.00000	0.00000	-0.31915	0.00000
10 Si	1 S	-0.62970	0.00000	0.00000	0.00000	-1.69680
11 Si	1 PX	0.00000	0.62114	-0.06644	0.00000	0.00000
12 Si	1 PY	0.00000	0.06644	0.62114	0.00000	0.00000
13 Si	1 PZ	0.00000	0.00000	0.00000	-0.77219	0.00000
14 Si	1 DXX	-0.06422	0.00000	0.00000	0.00000	0.12175
15 Si	1 DYY	-0.06422	0.00000	0.00000	0.00000	0.12175
16 Si	1 DZZ	-0.00729	0.00000	0.00000	0.00000	0.12565
17 Si	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18 Si	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 Si	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.48313	0.48313	0.51610	0.76232	0.76232
		A	A	A	A	A
1 Si	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 Si	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 Si	1 PX	-0.26083	-0.19935	0.00000	0.00000	0.00000
4 Si	1 PY	-0.19935	0.26083	0.00000	0.00000	0.00000
5 Si	1 PZ	0.00000	0.00000	-0.35771	0.00000	0.00000
6 Si	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 Si	1 PX	1.02668	0.78468	0.00000	0.00000	0.00000
8 Si	1 PY	0.78468	-1.02668	0.00000	0.00000	0.00000
9 Si	1 PZ	0.00000	0.00000	1.34481	0.00000	0.00000
10 Si	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 Si	1 PX	-0.93481	-0.71446	0.00000	0.00000	0.00000
12 Si	1 PY	-0.71446	0.93481	0.00000	0.00000	0.00000
13 Si	1 PZ	0.00000	0.00000	-1.08545	0.00000	0.00000
14 Si	1 DXX	0.00000	0.00000	0.00000	-0.86603	0.00037
15 Si	1 DYY	0.00000	0.00000	0.00000	0.86603	-0.00037
16 Si	1 DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
17 Si	1 DXY	0.00000	0.00000	0.00000	-0.00043	-1.00000
18 Si	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 Si	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		16	17	18	19
Eigenvalues:		0.78189	0.78189	0.78981	2.55863
		A	A	A	A
1 Si	1 S	0.00000	0.00000	0.00243	-0.13260
2 Si	1 S	0.00000	0.00000	-0.01341	1.05322
3 Si	1 PX	0.00000	0.00000	0.00000	0.00000
4 Si	1 PY	0.00000	0.00000	0.00000	0.00000
5 Si	1 PZ	0.00000	0.00000	0.00000	0.00000

6	Si	1	S	0.00000	0.00000	0.01404	-6.35082
7	Si	1	PX	0.00000	0.00000	0.00000	0.00000
8	Si	1	PY	0.00000	0.00000	0.00000	0.00000
9	Si	1	PZ	0.00000	0.00000	0.00000	0.00000
10	Si	1	S	0.00000	0.00000	0.02873	-0.54759
11	Si	1	PX	0.00000	0.00000	0.00000	0.00000
12	Si	1	PY	0.00000	0.00000	0.00000	0.00000
13	Si	1	PZ	0.00000	0.00000	0.00000	0.00000
14	Si	1	DXX	0.00000	0.00000	-0.50039	2.96209
15	Si	1	DYY	0.00000	0.00000	-0.50039	2.96209
16	Si	1	DZZ	0.00000	0.00000	0.99852	2.96317
17	Si	1	DXY	0.00000	0.00000	0.00000	0.00000
18	Si	1	DXZ	0.91606	0.40103	0.00000	0.00000
19	Si	1	DYZ	-0.40103	0.91606	0.00000	0.00000

Beta Spin Molecular Orbital Coefficients

MO:				1	2	3	4	5
Eigenvalues:				-68.38424	-6.12561	-4.22493	-4.21153	-4.21153
				A	A	A	A	A
1	Si	1	S	0.98617	0.28619	0.00000	0.00000	0.00000
2	Si	1	S	0.06078	-0.97116	0.00000	0.00000	0.00000
3	Si	1	PX	0.00000	0.00000	0.00000	0.97563	0.01407
4	Si	1	PY	0.00000	0.00000	0.00000	-0.01407	0.97563
5	Si	1	PZ	0.00000	0.00000	0.97503	0.00000	0.00000
6	Si	1	S	-0.10278	-0.31117	0.00000	0.00000	0.00000
7	Si	1	PX	0.00000	0.00000	0.00000	0.08487	0.00122
8	Si	1	PY	0.00000	0.00000	0.00000	-0.00122	0.08487
9	Si	1	PZ	0.00000	0.00000	0.08710	0.00000	0.00000
10	Si	1	S	-0.00350	0.01845	0.00000	0.00000	0.00000
11	Si	1	PX	0.00000	0.00000	0.00000	-0.02647	-0.00038
12	Si	1	PY	0.00000	0.00000	0.00000	0.00038	-0.02647
13	Si	1	PZ	0.00000	0.00000	-0.02702	0.00000	0.00000
14	Si	1	DXX	0.04264	0.09892	0.00000	0.00000	0.00000
15	Si	1	DYY	0.04264	0.09892	0.00000	0.00000	0.00000
16	Si	1	DZZ	0.04265	0.09770	0.00000	0.00000	0.00000
17	Si	1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Si	1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Si	1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:				6	7	8	9	10
Eigenvalues:				-0.45750	0.02912	0.07307	0.07307	0.44886
				A	A	A	A	A
1	Si	1	S	0.06722	0.00000	0.00000	0.00000	-0.05989
2	Si	1	S	-0.35229	0.00000	0.00000	0.00000	0.14535
3	Si	1	PX	0.00000	0.00000	-0.06429	0.15699	0.00000
4	Si	1	PY	0.00000	0.00000	-0.15699	-0.06429	0.00000
5	Si	1	PZ	0.00000	0.18130	0.00000	0.00000	0.00000
6	Si	1	S	0.40820	0.00000	0.00000	0.00000	-1.48817
7	Si	1	PX	0.00000	0.00000	0.10143	-0.24770	0.00000
8	Si	1	PY	0.00000	0.00000	0.24770	0.10143	0.00000
9	Si	1	PZ	0.00000	-0.30688	0.00000	0.00000	0.00000
10	Si	1	S	0.63214	0.00000	0.00000	0.00000	1.69868
11	Si	1	PX	0.00000	0.00000	0.30810	-0.75243	0.00000
12	Si	1	PY	0.00000	0.00000	0.75243	0.30810	0.00000
13	Si	1	PZ	0.00000	-0.78207	0.00000	0.00000	0.00000
14	Si	1	DXX	-0.00003	0.00000	0.00000	0.00000	-0.11027

```
15 Si  1 DYY      -0.00003    0.00000    0.00000    0.00000   -0.11027
16 Si  1 DZZ       0.05947    0.00000    0.00000    0.00000   -0.17048
17 Si  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
18 Si  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
19 Si  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000

MO:                  11         12         13         14         15

Eigenvalues:       0.52776    0.56639    0.56639    0.83567    0.84620

                      A          A          A          A          A
 1 Si  1 S         0.00000    0.00000    0.00000   -0.00547    0.00000
 2 Si  1 S         0.00000    0.00000    0.00000    0.02401    0.00000
 3 Si  1 PX        0.00000    0.00307    0.36306    0.00000    0.00000
 4 Si  1 PY        0.00000   -0.36306    0.00307    0.00000    0.00000
 5 Si  1 PZ       -0.35933    0.00000    0.00000    0.00000    0.00000
 6 Si  1 S         0.00000    0.00000    0.00000   -0.10630    0.00000
 7 Si  1 PX        0.00000   -0.01147   -1.35610    0.00000    0.00000
 8 Si  1 PY        0.00000    1.35610   -0.01147    0.00000    0.00000
 9 Si  1 PZ        1.34768    0.00000    0.00000    0.00000    0.00000
10 Si  1 S         0.00000    0.00000    0.00000    0.04066    0.00000
11 Si  1 PX        0.00000    0.00892    1.05515    0.00000    0.00000
12 Si  1 PY        0.00000   -1.05515    0.00892    0.00000    0.00000
13 Si  1 PZ       -1.07835    0.00000    0.00000    0.00000    0.00000
14 Si  1 DXX       0.00000    0.00000    0.00000   -0.49115    0.00000
15 Si  1 DYY       0.00000    0.00000    0.00000   -0.49115    0.00000
16 Si  1 DZZ       0.00000    0.00000    0.00000    1.00644    0.00000
17 Si  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
18 Si  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.08022
19 Si  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.99678

MO:                  16         17         18         19

Eigenvalues:       0.84620    0.88360    0.88360    2.58367

                      A          A          A          A
 1 Si  1 S         0.00000    0.00000    0.00000   -0.13226
 2 Si  1 S         0.00000    0.00000    0.00000    1.05105
 3 Si  1 PX        0.00000    0.00000    0.00000    0.00000
 4 Si  1 PY        0.00000    0.00000    0.00000    0.00000
 5 Si  1 PZ        0.00000    0.00000    0.00000    0.00000
 6 Si  1 S         0.00000    0.00000    0.00000   -6.35075
 7 Si  1 PX        0.00000    0.00000    0.00000    0.00000
 8 Si  1 PY        0.00000    0.00000    0.00000    0.00000
 9 Si  1 PZ        0.00000    0.00000    0.00000    0.00000
10 Si  1 S         0.00000    0.00000    0.00000   -0.53810
11 Si  1 PX        0.00000    0.00000    0.00000    0.00000
12 Si  1 PY        0.00000    0.00000    0.00000    0.00000
13 Si  1 PZ        0.00000    0.00000    0.00000    0.00000
14 Si  1 DXX       0.00000    0.86588    0.01586    2.96471
15 Si  1 DYY       0.00000   -0.86588   -0.01586    2.96471
16 Si  1 DZZ       0.00000    0.00000    0.00000    2.95763
17 Si  1 DXY       0.00000    0.01832   -0.99983    0.00000
18 Si  1 DXZ       0.99678    0.00000    0.00000    0.00000
19 Si  1 DYZ      -0.08022    0.00000    0.00000    0.00000

  ** Archive file written to unit 12 **

Total Cpu time:        0 mins.  1.13 secs.
Total Wall time:       0 mins.  1.87 secs.
```

```
  Calculation finished: Fri Sep 18 13:33:56 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:35:24 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  15
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  4

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    P  P1           0.0000000    -0.0828409    -0.2012426

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.76E-06 in   6 cycles  <S**2> = 3.7503

  E(HF)  =    -339.0595034 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -79.49806   -7.49719   -5.39139   -5.39139   -5.39139

                        A         A         A         A         A
   1 P   1 S        -0.98555   -0.29185    0.00000    0.00000    0.00000
   2 P   1 S        -0.06558    0.95589    0.00000    0.00000    0.00000
   3 P   1 PX        0.00000    0.00000   -0.32372   -0.91336    0.10237
   4 P   1 PY        0.00000    0.00000   -0.75871    0.20432   -0.57630
   5 P   1 PZ        0.00000    0.00000    0.51872   -0.27116   -0.77904
   6 P   1 S         0.09035    0.29890    0.00000    0.00000    0.00000
   7 P   1 PX        0.00000    0.00000   -0.02763   -0.07796    0.00874
   8 P   1 PY        0.00000    0.00000   -0.06476    0.01744   -0.04919
   9 P   1 PZ        0.00000    0.00000    0.04427   -0.02314   -0.06649
  10 P   1 S         0.00749   -0.00783    0.00000    0.00000    0.00000
  11 P   1 PX        0.00000    0.00000    0.00793    0.02237   -0.00251
  12 P   1 PY        0.00000    0.00000    0.01858   -0.00500    0.01411
  13 P   1 PZ        0.00000    0.00000   -0.01270    0.00664    0.01908
  14 P   1 DXX      -0.03791   -0.09122    0.00000    0.00000    0.00000
  15 P   1 DYY      -0.03791   -0.09122    0.00000    0.00000    0.00000
  16 P   1 DZZ      -0.03791   -0.09122    0.00000    0.00000    0.00000
  17 P   1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 P   1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 P   1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:			6	7	8	9	10
Eigenvalues:			-0.83174	-0.39072	-0.39072	-0.39072	0.49892
			A	A	A	A	A
1	P	1 S	0.07232	0.00000	0.00000	0.00000	0.06124
2	P	1 S	-0.38299	0.00000	0.00000	0.00000	-0.18407
3	P	1 PX	0.00000	-0.09532	0.21236	-0.10138	0.00000
4	P	1 PY	0.00000	-0.08243	-0.13258	-0.20023	0.00000
5	P	1 PZ	0.00000	-0.22041	-0.04226	0.11872	0.00000
6	P	1 S	0.38417	0.00000	0.00000	0.00000	1.45438
7	P	1 PX	0.00000	0.20003	-0.44565	0.21275	0.00000
8	P	1 PY	0.00000	0.17297	0.27823	0.42018	0.00000
9	P	1 PZ	0.00000	0.46254	0.08868	-0.24913	0.00000
10	P	1 S	0.60351	0.00000	0.00000	0.00000	-1.76987
11	P	1 PX	0.00000	0.22171	-0.49395	0.23581	0.00000
12	P	1 PY	0.00000	0.19172	0.30839	0.46572	0.00000
13	P	1 PZ	0.00000	0.51268	0.09829	-0.27614	0.00000
14	P	1 DXX	0.04601	0.00000	0.00000	0.00000	0.17820
15	P	1 DYY	0.04601	0.00000	0.00000	0.00000	0.17820
16	P	1 DZZ	0.04601	0.00000	0.00000	0.00000	0.17820
17	P	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	P	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	P	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:			11	12	13	14	15
Eigenvalues:			0.59843	0.59843	0.59843	0.84704	0.84704
			A	A	A	A	A
1	P	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2	P	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3	P	1 PX	0.08726	0.29185	0.15998	0.00000	0.00000
4	P	1 PY	-0.33013	0.05492	0.07987	0.00000	0.00000
5	P	1 PZ	-0.04222	0.17376	-0.29395	0.00000	0.00000
6	P	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7	P	1 PX	-0.32523	-1.08776	-0.59628	0.00000	0.00000
8	P	1 PY	1.23046	-0.20470	-0.29771	0.00000	0.00000
9	P	1 PZ	0.15734	-0.64762	1.09562	0.00000	0.00000
10	P	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11	P	1 PX	0.30207	1.01030	0.55382	0.00000	0.00000
12	P	1 PY	-1.14283	0.19012	0.27651	0.00000	0.00000
13	P	1 PZ	-0.14614	0.60151	-1.01760	0.00000	0.00000
14	P	1 DXX	0.00000	0.00000	0.00000	-0.87872	-0.41476
15	P	1 DYY	0.00000	0.00000	0.00000	0.07475	0.95309
16	P	1 DZZ	0.00000	0.00000	0.00000	0.80397	-0.53833
17	P	1 DXY	0.00000	0.00000	0.00000	0.17499	-0.06305
18	P	1 DXZ	0.00000	0.00000	0.00000	-0.10809	-0.22964
19	P	1 DYZ	0.00000	0.00000	0.00000	-0.09105	0.17266

MO:			16	17	18	19
Eigenvalues:			0.84704	0.84704	0.84704	2.98713
			A	A	A	A
1	P	1 S	0.00000	0.00000	0.00000	-0.12648
2	P	1 S	0.00000	0.00000	0.00000	1.22438
3	P	1 PX	0.00000	0.00000	0.00000	0.00000
4	P	1 PY	0.00000	0.00000	0.00000	0.00000
5	P	1 PZ	0.00000	0.00000	0.00000	0.00000

6	P	1	S	0.00000	0.00000	0.00000	-5.38844
7	P	1	PX	0.00000	0.00000	0.00000	0.00000
8	P	1	PY	0.00000	0.00000	0.00000	0.00000
9	P	1	PZ	0.00000	0.00000	0.00000	0.00000
10	P	1	S	0.00000	0.00000	0.00000	-0.83712
11	P	1	PX	0.00000	0.00000	0.00000	0.00000
12	P	1	PY	0.00000	0.00000	0.00000	0.00000
13	P	1	PZ	0.00000	0.00000	0.00000	0.00000
14	P	1	DXX	-0.11082	0.11867	-0.17163	2.61804
15	P	1	DYY	0.26911	-0.11388	-0.02522	2.61804
16	P	1	DZZ	-0.15829	-0.00479	0.19685	2.61804
17	P	1	DXY	0.42631	0.71129	-0.52701	0.00000
18	P	1	DXZ	0.82991	-0.13743	0.47743	0.00000
19	P	1	DYZ	-0.23735	0.67612	0.66964	0.00000

Beta Spin Molecular Orbital Coefficients

MO:				1	2	3	4	5
Eigenvalues:				-79.47896	-7.47620	-5.35247	-5.35247	-5.35247
				A	A	A	A	A
1	P	1	S	-0.98562	-0.29182	0.00000	0.00000	0.00000
2	P	1	S	-0.06528	0.95601	0.00000	0.00000	0.00000
3	P	1	PX	0.00000	0.00000	0.17143	0.90640	0.31230
4	P	1	PY	0.00000	0.00000	0.95607	-0.18511	0.01244
5	P	1	PZ	0.00000	0.00000	0.07094	0.30439	-0.92239
6	P	1	S	0.08978	0.30182	0.00000	0.00000	0.00000
7	P	1	PX	0.00000	0.00000	0.01496	0.07912	0.02726
8	P	1	PY	0.00000	0.00000	0.08346	-0.01616	0.00109
9	P	1	PZ	0.00000	0.00000	0.00619	0.02657	-0.08052
10	P	1	S	0.00744	-0.00819	0.00000	0.00000	0.00000
11	P	1	PX	0.00000	0.00000	-0.00446	-0.02359	-0.00813
12	P	1	PY	0.00000	0.00000	-0.02488	0.00482	-0.00032
13	P	1	PZ	0.00000	0.00000	-0.00185	-0.00792	0.02401
14	P	1	DXX	-0.03770	-0.09362	0.00000	0.00000	0.00000
15	P	1	DYY	-0.03770	-0.09362	0.00000	0.00000	0.00000
16	P	1	DZZ	-0.03770	-0.09362	0.00000	0.00000	0.00000
17	P	1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	P	1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	P	1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:				6	7	8	9	10
Eigenvalues:				-0.55220	0.06476	0.06476	0.06476	0.56726
				A	A	A	A	A
1	P	1	S	-0.07206	0.00000	0.00000	0.00000	0.06121
2	P	1	S	0.39158	0.00000	0.00000	0.00000	-0.18133
3	P	1	PX	0.00000	0.05921	0.18371	0.03481	0.00000
4	P	1	PY	0.00000	0.16421	-0.03363	-0.10184	0.00000
5	P	1	PZ	0.00000	-0.08942	0.05988	-0.16396	0.00000
6	P	1	S	-0.42720	0.00000	0.00000	0.00000	1.42865
7	P	1	PX	0.00000	-0.09743	-0.30232	-0.05728	0.00000
8	P	1	PY	0.00000	-0.27022	0.05534	0.16758	0.00000
9	P	1	PZ	0.00000	0.14715	-0.09855	0.26982	0.00000
10	P	1	S	-0.63345	0.00000	0.00000	0.00000	-1.76729
11	P	1	PX	0.00000	-0.23302	-0.72304	-0.13699	0.00000
12	P	1	PY	0.00000	-0.64629	0.13235	0.40081	0.00000
13	P	1	PZ	0.00000	0.35194	-0.23569	0.64532	0.00000
14	P	1	DXX	-0.01481	0.00000	0.00000	0.00000	0.19340

15 P	1 DYY	-0.01481	0.00000	0.00000	0.00000	0.19340
16 P	1 DZZ	-0.01481	0.00000	0.00000	0.00000	0.19340
17 P	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18 P	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 P	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.70045	0.70045	0.70045	0.99961	0.99961
		A	A	A	A	A
1 P	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 P	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 P	1 PX	0.01386	-0.30373	-0.23010	0.00000	0.00000
4 P	1 PY	-0.33208	0.10329	-0.15634	0.00000	0.00000
5 P	1 PZ	-0.18687	-0.20608	0.26077	0.00000	0.00000
6 P	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 P	1 PX	-0.04909	1.07578	0.81501	0.00000	0.00000
8 P	1 PY	1.17621	-0.36585	0.55375	0.00000	0.00000
9 P	1 PZ	0.66188	0.72994	-0.92361	0.00000	0.00000
10 P	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 P	1 PX	0.03934	-0.86216	-0.65317	0.00000	0.00000
12 P	1 PY	-0.94264	0.29320	-0.44379	0.00000	0.00000
13 P	1 PZ	-0.53045	-0.58499	0.74021	0.00000	0.00000
14 P	1 DXX	0.00000	0.00000	0.00000	0.55995	0.52978
15 P	1 DYY	0.00000	0.00000	0.00000	0.12565	-0.70461
16 P	1 DZZ	0.00000	0.00000	0.00000	-0.68560	0.17483
17 P	1 DXY	0.00000	0.00000	0.00000	-0.11360	0.45598
18 P	1 DXZ	0.00000	0.00000	0.00000	0.66396	-0.09656
19 P	1 DYZ	0.00000	0.00000	0.00000	-0.11548	-0.49426

MO:		16	17	18	19
Eigenvalues:		0.99961	0.99961	0.99961	3.03457
		A	A	A	A
1 P	1 S	0.00000	0.00000	0.00000	0.12619
2 P	1 S	0.00000	0.00000	0.00000	-1.22199
3 P	1 PX	0.00000	0.00000	0.00000	0.00000
4 P	1 PY	0.00000	0.00000	0.00000	0.00000
5 P	1 PZ	0.00000	0.00000	0.00000	0.00000
6 P	1 S	0.00000	0.00000	0.00000	5.39193
7 P	1 PX	0.00000	0.00000	0.00000	0.00000
8 P	1 PY	0.00000	0.00000	0.00000	0.00000
9 P	1 PZ	0.00000	0.00000	0.00000	0.00000
10 P	1 S	0.00000	0.00000	0.00000	0.82029
11 P	1 PX	0.00000	0.00000	0.00000	0.00000
12 P	1 PY	0.00000	0.00000	0.00000	0.00000
13 P	1 PZ	0.00000	0.00000	0.00000	0.00000
14 P	1 DXX	0.45072	0.44798	-0.04428	-2.61724
15 P	1 DYY	-0.66054	0.22623	0.01577	-2.61724
16 P	1 DZZ	0.20982	-0.67421	0.02851	-2.61724
17 P	1 DXY	-0.44677	0.12647	0.75072	0.00000
18 P	1 DXZ	0.00005	-0.68857	0.27515	0.00000
19 P	1 DYZ	0.58715	0.19732	0.59891	0.00000

** Archive file written to unit 12 **

Total Cpu time: 0 mins. 1.27 secs.
Total Wall time: 0 mins. 1.82 secs.

```
  Calculation finished: Fri Sep 18 13:35:26 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:36:39 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  16
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  3

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    S  S1          -0.0000001     1.7810652    -2.3970894

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.64E-05 in   5 cycles  <S**2> = 2.0055

  E(HF)  =    -395.6312238 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -91.46990   -8.98266   -6.67271   -6.67271   -6.65101

                        A         A         A         A         A
   1 S   1 S        -0.98493   -0.29739    0.00000    0.00000    0.00000
   2 S   1 S        -0.07343    0.93682    0.00000    0.00000    0.00000
   3 S   1 PX        0.00000    0.00000    0.00000    0.00000   -0.97517
   4 S   1 PY        0.00000    0.00000   -0.83243    0.50691    0.00000
   5 S   1 PZ        0.00000    0.00000   -0.50691   -0.83243    0.00000
   6 S   1 S         0.09582    0.30808    0.00000    0.00000    0.00000
   7 S   1 PX        0.00000    0.00000    0.00000    0.00000   -0.07814
   8 S   1 PY        0.00000    0.00000   -0.06807    0.04145    0.00000
   9 S   1 PZ        0.00000    0.00000   -0.04145   -0.06807    0.00000
  10 S   1 S         0.00585   -0.01306    0.00000    0.00000    0.00000
  11 S   1 PX        0.00000    0.00000    0.00000    0.00000    0.02225
  12 S   1 PY        0.00000    0.00000    0.01932   -0.01176    0.00000
  13 S   1 PZ        0.00000    0.00000    0.01176    0.01932    0.00000
  14 S   1 DXX      -0.03853   -0.09007    0.00000    0.00000    0.00000
  15 S   1 DYY      -0.03853   -0.08881    0.00000    0.00000    0.00000
  16 S   1 DZZ      -0.03853   -0.08881    0.00000    0.00000    0.00000
  17 S   1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 S   1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 S   1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:		6	7	8	9	10
Eigenvalues:		-0.98274	-0.48109	-0.48109	-0.41504	0.53459
		A	A	A	A	A
1 S	1 S	-0.07712	0.00000	0.00000	0.00000	-0.05981
2 S	1 S	0.43215	0.00000	0.00000	0.00000	0.26995
3 S	1 PX	0.00000	0.00000	0.00000	-0.26873	0.00000
4 S	1 PY	0.00000	-0.00022	-0.27749	0.00000	0.00000
5 S	1 PZ	0.00000	-0.27749	0.00022	0.00000	0.00000
6 S	1 S	-0.50997	0.00000	0.00000	0.00000	-1.46902
7 S	1 PX	0.00000	0.00000	0.00000	0.58273	0.00000
8 S	1 PY	0.00000	0.00049	0.61065	0.00000	0.00000
9 S	1 PZ	0.00000	0.61065	-0.00049	0.00000	0.00000
10 S	1 S	-0.51939	0.00000	0.00000	0.00000	1.77924
11 S	1 PX	0.00000	0.00000	0.00000	0.55065	0.00000
12 S	1 PY	0.00000	0.00042	0.52363	0.00000	0.00000
13 S	1 PZ	0.00000	0.52363	-0.00042	0.00000	0.00000
14 S	1 DXX	-0.00241	0.00000	0.00000	0.00000	-0.13043
15 S	1 DYY	-0.05144	0.00000	0.00000	0.00000	-0.18658
16 S	1 DZZ	-0.05144	0.00000	0.00000	0.00000	-0.18658
17 S	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18 S	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 S	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.64719	0.64719	0.69137	0.92255	0.92255
		A	A	A	A	A
1 S	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 S	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 S	1 PX	0.00000	0.00000	-0.34485	0.00000	0.00000
4 S	1 PY	-0.00237	-0.33939	0.00000	0.00000	0.00000
5 S	1 PZ	0.33939	-0.00237	0.00000	0.00000	0.00000
6 S	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 S	1 PX	0.00000	0.00000	1.23969	0.00000	0.00000
8 S	1 PY	0.00858	1.22604	0.00000	0.00000	0.00000
9 S	1 PZ	-1.22604	0.00858	0.00000	0.00000	0.00000
10 S	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 S	1 PX	0.00000	0.00000	-1.18442	0.00000	0.00000
12 S	1 PY	-0.00837	-1.19657	0.00000	0.00000	0.00000
13 S	1 PZ	1.19657	-0.00837	0.00000	0.00000	0.00000
14 S	1 DXX	0.00000	0.00000	0.00000	0.00000	0.00000
15 S	1 DYY	0.00000	0.00000	0.00000	0.86601	-0.00515
16 S	1 DZZ	0.00000	0.00000	0.00000	-0.86601	0.00515
17 S	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18 S	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 S	1 DYZ	0.00000	0.00000	0.00000	-0.00595	-0.99998

MO:		16	17	18	19
Eigenvalues:		0.97214	0.97214	0.99084	3.68119
		A	A	A	A
1 S	1 S	0.00000	0.00000	-0.00498	-0.12283
2 S	1 S	0.00000	0.00000	0.02925	1.51009
3 S	1 PX	0.00000	0.00000	0.00000	0.00000
4 S	1 PY	0.00000	0.00000	0.00000	0.00000
5 S	1 PZ	0.00000	0.00000	0.00000	0.00000

6	S	1	S	0.00000	0.00000	-0.09230	-5.29992
7	S	1	PX	0.00000	0.00000	0.00000	0.00000
8	S	1	PY	0.00000	0.00000	0.00000	0.00000
9	S	1	PZ	0.00000	0.00000	0.00000	0.00000
10	S	1	S	0.00000	0.00000	0.04688	-0.73541
11	S	1	PX	0.00000	0.00000	0.00000	0.00000
12	S	1	PY	0.00000	0.00000	0.00000	0.00000
13	S	1	PZ	0.00000	0.00000	0.00000	0.00000
14	S	1	DXX	0.00000	0.00000	-0.99658	2.49594
15	S	1	DYY	0.00000	0.00000	0.50156	2.49021
16	S	1	DZZ	0.00000	0.00000	0.50156	2.49021
17	S	1	DXY	0.35154	0.93617	0.00000	0.00000
18	S	1	DXZ	0.93617	-0.35154	0.00000	0.00000
19	S	1	DYZ	0.00000	0.00000	0.00000	0.00000

Beta Spin Molecular Orbital Coefficients

MO:				1	2	3	4	5
Eigenvalues:				-91.45242	-8.96454	-6.64165	-6.62754	-6.62754
				A	A	A	A	A
1	S	1	S	-0.98498	-0.29739	0.00000	0.00000	0.00000
2	S	1	S	-0.07317	0.93691	0.00000	0.00000	0.00000
3	S	1	PX	0.00000	0.00000	-0.97528	0.00000	0.00000
4	S	1	PY	0.00000	0.00000	0.00000	0.11089	-0.96764
5	S	1	PZ	0.00000	0.00000	0.00000	-0.96764	-0.11089
6	S	1	S	0.09537	0.30972	0.00000	0.00000	0.00000
7	S	1	PX	0.00000	0.00000	-0.07786	0.00000	0.00000
8	S	1	PY	0.00000	0.00000	0.00000	0.00931	-0.08126
9	S	1	PZ	0.00000	0.00000	0.00000	-0.08126	-0.00931
10	S	1	S	0.00582	-0.01324	0.00000	0.00000	0.00000
11	S	1	PX	0.00000	0.00000	0.02240	0.00000	0.00000
12	S	1	PY	0.00000	0.00000	0.00000	-0.00273	0.02381
13	S	1	PZ	0.00000	0.00000	0.00000	0.02381	0.00273
14	S	1	DXX	-0.03834	-0.09059	0.00000	0.00000	0.00000
15	S	1	DYY	-0.03837	-0.09090	0.00000	0.00000	0.00000
16	S	1	DZZ	-0.03837	-0.09090	0.00000	0.00000	0.00000
17	S	1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	S	1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	S	1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:				6	7	8	9	10
Eigenvalues:				-0.76857	-0.37197	0.01778	0.01778	0.58358
				A	A	A	A	A
1	S	1	S	0.07618	0.00000	0.00000	0.00000	0.06043
2	S	1	S	-0.43422	0.00000	0.00000	0.00000	-0.27044
3	S	1	PX	0.00000	0.26362	0.00000	0.00000	0.00000
4	S	1	PY	0.00000	0.00000	0.03855	0.21743	0.00000
5	S	1	PZ	0.00000	0.00000	-0.21743	0.03855	0.00000
6	S	1	S	0.51739	0.00000	0.00000	0.00000	1.45618
7	S	1	PX	0.00000	-0.56575	0.00000	0.00000	0.00000
8	S	1	PY	0.00000	0.00000	-0.07148	-0.40315	0.00000
9	S	1	PZ	0.00000	0.00000	0.40315	-0.07148	0.00000
10	S	1	S	0.54934	0.00000	0.00000	0.00000	-1.77505
11	S	1	PX	0.00000	-0.56679	0.00000	0.00000	0.00000
12	S	1	PY	0.00000	0.00000	-0.12325	-0.69511	0.00000
13	S	1	PZ	0.00000	0.00000	0.69511	-0.12325	0.00000
14	S	1	DXX	0.05742	0.00000	0.00000	0.00000	0.17974

```
15 S   1 DYY      -0.00022    0.00000    0.00000    0.00000    0.17833
16 S   1 DZZ      -0.00022    0.00000    0.00000    0.00000    0.17833
17 S   1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
18 S   1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
19 S   1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000

MO:                  11         12         13         14         15

Eigenvalues:       0.70921    0.75206    0.75206    1.05817    1.06550

                       A          A          A          A          A
 1 S   1 S         0.00000    0.00000    0.00000   -0.00292    0.00000
 2 S   1 S         0.00000    0.00000    0.00000    0.01693    0.00000
 3 S   1 PX       -0.34844    0.00000    0.00000    0.00000    0.00000
 4 S   1 PY        0.00000   -0.02566   -0.37952    0.00000    0.00000
 5 S   1 PZ        0.00000    0.37952   -0.02566    0.00000    0.00000
 6 S   1 S         0.00000    0.00000    0.00000   -0.02194    0.00000
 7 S   1 PX        1.24755    0.00000    0.00000    0.00000    0.00000
 8 S   1 PY        0.00000    0.08816    1.30400    0.00000    0.00000
 9 S   1 PZ        0.00000   -1.30400    0.08816    0.00000    0.00000
10 S   1 S         0.00000    0.00000    0.00000   -0.01953    0.00000
11 S   1 PX       -1.17678    0.00000    0.00000    0.00000    0.00000
12 S   1 PY        0.00000   -0.07412   -1.09641    0.00000    0.00000
13 S   1 PZ        0.00000    1.09641   -0.07412    0.00000    0.00000
14 S   1 DXX       0.00000    0.00000    0.00000    0.99867    0.00000
15 S   1 DYY       0.00000    0.00000    0.00000   -0.50023    0.00000
16 S   1 DZZ       0.00000    0.00000    0.00000   -0.50023    0.00000
17 S   1 DXY       0.00000    0.00000    0.00000    0.00000    1.00000
18 S   1 DXZ       0.00000    0.00000    0.00000    0.00000   -0.00172
19 S   1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000

MO:                  16         17         18         19

Eigenvalues:       1.06550    1.09319    1.09319    3.71995

                       A          A          A          A
 1 S   1 S         0.00000    0.00000    0.00000   -0.12279
 2 S   1 S         0.00000    0.00000    0.00000    1.50955
 3 S   1 PX        0.00000    0.00000    0.00000    0.00000
 4 S   1 PY        0.00000    0.00000    0.00000    0.00000
 5 S   1 PZ        0.00000    0.00000    0.00000    0.00000
 6 S   1 S         0.00000    0.00000    0.00000   -5.30341
 7 S   1 PX        0.00000    0.00000    0.00000    0.00000
 8 S   1 PY        0.00000    0.00000    0.00000    0.00000
 9 S   1 PZ        0.00000    0.00000    0.00000    0.00000
10 S   1 S         0.00000    0.00000    0.00000   -0.72494
11 S   1 PX        0.00000    0.00000    0.00000    0.00000
12 S   1 PY        0.00000    0.00000    0.00000    0.00000
13 S   1 PZ        0.00000    0.00000    0.00000    0.00000
14 S   1 DXX       0.00000    0.00000    0.00000    2.49137
15 S   1 DYY       0.00000   -0.82955   -0.24870    2.49154
16 S   1 DZZ       0.00000    0.82955    0.24870    2.49154
17 S   1 DXY      -0.00172    0.00000    0.00000    0.00000
18 S   1 DXZ      -1.00000    0.00000    0.00000    0.00000
19 S   1 DYZ       0.00000    0.28717   -0.95788    0.00000

  ** Archive file written to unit 12 **

Total Cpu time:        0 mins.  1.14 secs.
Total Wall time:       0 mins.  1.83 secs.
```

```
  Calculation finished: Fri Sep 18 13:36:41 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:37:55 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  17
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Cl Cl1          0.0000000     2.8994087    -2.1997787

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.57E-06 in   6 cycles  <S**2> = 0.7549

  E(HF)  =    -457.3710925 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:    -104.27722  -10.57914   -8.06308   -8.03739   -8.03739

                        A         A         A         A         A
   1 Cl  1 S         0.98445    0.30207    0.00000    0.00000    0.00000
   2 Cl  1 S         0.07571   -0.92852    0.00000    0.00000    0.00000
   3 Cl  1 PX        0.00000    0.00000    0.00000    0.92111   -0.32020
   4 Cl  1 PY        0.00000    0.00000    0.00000    0.32020    0.92111
   5 Cl  1 PZ        0.00000    0.00000    0.97467    0.00000    0.00000
   6 Cl  1 S        -0.08954   -0.30472    0.00000    0.00000    0.00000
   7 Cl  1 PX        0.00000    0.00000    0.00000    0.07200   -0.02503
   8 Cl  1 PY        0.00000    0.00000    0.00000    0.02503    0.07200
   9 Cl  1 PZ        0.00000    0.00000    0.07767    0.00000    0.00000
  10 Cl  1 S        -0.00600    0.01230    0.00000    0.00000    0.00000
  11 Cl  1 PX        0.00000    0.00000    0.00000   -0.02049    0.00712
  12 Cl  1 PY        0.00000    0.00000    0.00000   -0.00712   -0.02049
  13 Cl  1 PZ        0.00000    0.00000   -0.02204    0.00000    0.00000
  14 Cl  1 DXX       0.03542    0.08603    0.00000    0.00000    0.00000
  15 Cl  1 DYY       0.03542    0.08603    0.00000    0.00000    0.00000
  16 Cl  1 DZZ       0.03541    0.08479    0.00000    0.00000    0.00000
  17 Cl  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 Cl  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 Cl  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:		6	7	8	9	10
Eigenvalues:		-1.12948	-0.57434	-0.50070	-0.50070	0.60324
		A	A	A	A	A
1 Cl	1 S	-0.08078	0.00000	0.00000	0.00000	-0.05894
2 Cl	1 S	0.46419	0.00000	0.00000	0.00000	0.29229
3 Cl	1 PX	0.00000	0.00000	0.04711	0.28231	0.00000
4 Cl	1 PY	0.00000	0.00000	0.28231	-0.04711	0.00000
5 Cl	1 PZ	0.00000	-0.29459	0.00000	0.00000	0.00000
6 Cl	1 S	-0.57372	0.00000	0.00000	0.00000	-1.43204
7 Cl	1 PX	0.00000	0.00000	-0.10421	-0.62445	0.00000
8 Cl	1 PY	0.00000	0.00000	-0.62445	0.10421	0.00000
9 Cl	1 PZ	0.00000	0.65936	0.00000	0.00000	0.00000
10 Cl	1 S	-0.47422	0.00000	0.00000	0.00000	1.81039
11 Cl	1 PX	0.00000	0.00000	-0.08319	-0.49851	0.00000
12 Cl	1 PY	0.00000	0.00000	-0.49851	0.08319	0.00000
13 Cl	1 PZ	0.00000	0.47912	0.00000	0.00000	0.00000
14 Cl	1 DXX	-0.01499	0.00000	0.00000	0.00000	-0.17217
15 Cl	1 DYY	-0.01499	0.00000	0.00000	0.00000	-0.17217
16 Cl	1 DZZ	-0.06429	0.00000	0.00000	0.00000	-0.23258
17 Cl	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18 Cl	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 Cl	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.72140	0.76797	0.76797	1.04276	1.05860
		A	A	A	A	A
1 Cl	1 S	0.00000	0.00000	0.00000	-0.00521	0.00000
2 Cl	1 S	0.00000	0.00000	0.00000	0.03176	0.00000
3 Cl	1 PX	0.00000	0.31762	-0.12947	0.00000	0.00000
4 Cl	1 PY	0.00000	0.12947	0.31762	0.00000	0.00000
5 Cl	1 PZ	0.33731	0.00000	0.00000	0.00000	0.00000
6 Cl	1 S	0.00000	0.00000	0.00000	-0.09392	0.00000
7 Cl	1 PX	0.00000	-1.12045	0.45671	0.00000	0.00000
8 Cl	1 PY	0.00000	-0.45671	-1.12045	0.00000	0.00000
9 Cl	1 PZ	-1.19575	0.00000	0.00000	0.00000	0.00000
10 Cl	1 S	0.00000	0.00000	0.00000	0.05474	0.00000
11 Cl	1 PX	0.00000	1.10732	-0.45136	0.00000	0.00000
12 Cl	1 PY	0.00000	0.45136	1.10732	0.00000	0.00000
13 Cl	1 PZ	1.20654	0.00000	0.00000	0.00000	0.00000
14 Cl	1 DXX	0.00000	0.00000	0.00000	-0.49999	0.00000
15 Cl	1 DYY	0.00000	0.00000	0.00000	-0.49999	0.00000
16 Cl	1 DZZ	0.00000	0.00000	0.00000	0.99797	0.00000
17 Cl	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18 Cl	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.27413
19 Cl	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.96169

MO:		16	17	18	19
Eigenvalues:		1.05860	1.11342	1.11342	4.22848
		A	A	A	A
1 Cl	1 S	0.00000	0.00000	0.00000	-0.12134
2 Cl	1 S	0.00000	0.00000	0.00000	1.55946
3 Cl	1 PX	0.00000	0.00000	0.00000	0.00000
4 Cl	1 PY	0.00000	0.00000	0.00000	0.00000
5 Cl	1 PZ	0.00000	0.00000	0.00000	0.00000

6	Cl	1	S	0.00000	0.00000	0.00000	-4.86092
7	Cl	1	PX	0.00000	0.00000	0.00000	0.00000
8	Cl	1	PY	0.00000	0.00000	0.00000	0.00000
9	Cl	1	PZ	0.00000	0.00000	0.00000	0.00000
10	Cl	1	S	0.00000	0.00000	0.00000	-0.76365
11	Cl	1	PX	0.00000	0.00000	0.00000	0.00000
12	Cl	1	PY	0.00000	0.00000	0.00000	0.00000
13	Cl	1	PZ	0.00000	0.00000	0.00000	0.00000
14	Cl	1	DXX	0.00000	-0.76785	-0.40051	2.29859
15	Cl	1	DYY	0.00000	0.76785	0.40051	2.29859
16	Cl	1	DZZ	0.00000	0.00000	0.00000	2.29334
17	Cl	1	DXY	0.00000	0.46247	-0.88664	0.00000
18	Cl	1	DXZ	0.96169	0.00000	0.00000	0.00000
19	Cl	1	DYZ	-0.27413	0.00000	0.00000	0.00000

Beta Spin Molecular Orbital Coefficients

MO:				1	2	3	4	5
Eigenvalues:				-104.26611	-10.56813	-8.03157	-8.03157	-8.01430
				A	A	A	A	A
1	Cl	1	S	-0.98448	-0.30208	0.00000	0.00000	0.00000
2	Cl	1	S	-0.07557	0.92866	0.00000	0.00000	0.00000
3	Cl	1	PX	0.00000	0.00000	-0.96880	0.11201	0.00000
4	Cl	1	PY	0.00000	0.00000	0.11201	0.96880	0.00000
5	Cl	1	PZ	0.00000	0.00000	0.00000	0.00000	0.97390
6	Cl	1	S	0.08931	0.30516	0.00000	0.00000	0.00000
7	Cl	1	PX	0.00000	0.00000	-0.07556	0.00874	0.00000
8	Cl	1	PY	0.00000	0.00000	0.00874	0.07556	0.00000
9	Cl	1	PZ	0.00000	0.00000	0.00000	0.00000	0.08003
10	Cl	1	S	0.00599	-0.01233	0.00000	0.00000	0.00000
11	Cl	1	PX	0.00000	0.00000	0.02161	-0.00250	0.00000
12	Cl	1	PY	0.00000	0.00000	-0.00250	-0.02161	0.00000
13	Cl	1	PZ	0.00000	0.00000	0.00000	0.00000	-0.02331
14	Cl	1	DXX	-0.03532	-0.08616	0.00000	0.00000	0.00000
15	Cl	1	DYY	-0.03532	-0.08616	0.00000	0.00000	0.00000
16	Cl	1	DZZ	-0.03535	-0.08658	0.00000	0.00000	0.00000
17	Cl	1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Cl	1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Cl	1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:				6	7	8	9	10
Eigenvalues:				-1.00854	-0.47598	-0.47598	-0.03535	0.62921
				A	A	A	A	A
1	Cl	1	S	0.08009	0.00000	0.00000	0.00000	0.05947
2	Cl	1	S	-0.46357	0.00000	0.00000	0.00000	-0.29360
3	Cl	1	PX	0.00000	-0.05463	0.27802	0.00000	0.00000
4	Cl	1	PY	0.00000	-0.27802	-0.05463	0.00000	0.00000
5	Cl	1	PZ	0.00000	0.00000	0.00000	0.24283	0.00000
6	Cl	1	S	0.57066	0.00000	0.00000	0.00000	1.42796
7	Cl	1	PX	0.00000	0.12026	-0.61198	0.00000	0.00000
8	Cl	1	PY	0.00000	0.61198	0.12026	0.00000	0.00000
9	Cl	1	PZ	0.00000	0.00000	0.00000	-0.47736	0.00000
10	Cl	1	S	0.49258	0.00000	0.00000	0.00000	-1.80854
11	Cl	1	PX	0.00000	0.09924	-0.50501	0.00000	0.00000
12	Cl	1	PY	0.00000	0.50501	0.09924	0.00000	0.00000
13	Cl	1	PZ	0.00000	0.00000	0.00000	-0.65041	0.00000
14	Cl	1	DXX	0.04265	0.00000	0.00000	0.00000	0.19950

```
15 Cl  1 DYY       0.04265    0.00000    0.00000    0.00000    0.19950
16 Cl  1 DZZ      -0.01093    0.00000    0.00000    0.00000    0.19531
17 Cl  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
18 Cl  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
19 Cl  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000

MO:                  11         12         13         14         15

Eigenvalues:       0.77794    0.77794    0.82442    1.12312    1.12312

                       A          A          A          A          A
 1 Cl  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
 2 Cl  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
 3 Cl  1 PX        0.34513    0.00535    0.00000    0.00000    0.00000
 4 Cl  1 PY       -0.00535    0.34513    0.00000    0.00000    0.00000
 5 Cl  1 PZ        0.00000    0.00000    0.37828    0.00000    0.00000
 6 Cl  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
 7 Cl  1 PX       -1.21469   -0.01883    0.00000    0.00000    0.00000
 8 Cl  1 PY        0.01883   -1.21469    0.00000    0.00000    0.00000
 9 Cl  1 PZ        0.00000    0.00000   -1.27919    0.00000    0.00000
10 Cl  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
11 Cl  1 PX        1.19167    0.01847    0.00000    0.00000    0.00000
12 Cl  1 PY       -0.01847    1.19167    0.00000    0.00000    0.00000
13 Cl  1 PZ        0.00000    0.00000    1.12347    0.00000    0.00000
14 Cl  1 DXX       0.00000    0.00000    0.00000    0.86125    0.09086
15 Cl  1 DYY       0.00000    0.00000    0.00000   -0.86125   -0.09086
16 Cl  1 DZZ       0.00000    0.00000    0.00000    0.00000    0.00000
17 Cl  1 DXY       0.00000    0.00000    0.00000    0.10491   -0.99448
18 Cl  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
19 Cl  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000

MO:                  16         17         18         19

Eigenvalues:       1.15556    1.15556    1.16843    4.25150

                       A          A          A          A
 1 Cl  1 S         0.00000    0.00000   -0.00290   -0.12137
 2 Cl  1 S         0.00000    0.00000    0.01684    1.55955
 3 Cl  1 PX        0.00000    0.00000    0.00000    0.00000
 4 Cl  1 PY        0.00000    0.00000    0.00000    0.00000
 5 Cl  1 PZ        0.00000    0.00000    0.00000    0.00000
 6 Cl  1 S         0.00000    0.00000   -0.02355   -4.86331
 7 Cl  1 PX        0.00000    0.00000    0.00000    0.00000
 8 Cl  1 PY        0.00000    0.00000    0.00000    0.00000
 9 Cl  1 PZ        0.00000    0.00000    0.00000    0.00000
10 Cl  1 S         0.00000    0.00000   -0.01241   -0.75824
11 Cl  1 PX        0.00000    0.00000    0.00000    0.00000
12 Cl  1 PY        0.00000    0.00000    0.00000    0.00000
13 Cl  1 PZ        0.00000    0.00000    0.00000    0.00000
14 Cl  1 DXX       0.00000    0.00000    0.49783    2.29649
15 Cl  1 DYY       0.00000    0.00000    0.49783    2.29649
16 Cl  1 DZZ       0.00000    0.00000   -1.00121    2.29621
17 Cl  1 DXY       0.00000    0.00000    0.00000    0.00000
18 Cl  1 DXZ      -0.01914   -0.99982    0.00000    0.00000
19 Cl  1 DYZ       0.99982   -0.01914    0.00000    0.00000

  ** Archive file written to unit 12 **

Total Cpu time:        0 mins.  1.28 secs.
Total Wall time:       0 mins.  1.71 secs.
```

```
  Calculation finished: Fri Sep 18 13:37:57 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:39:35 1998

  Run type: Single point energy
  Model: RHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  18
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Ar Ar1         -0.0000001    -0.3934908    -1.9923078

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  RHF direct SCF procedure requested

  Energy converged to 0.33E-11 in  12 cycles

  E(HF)  =    -524.4475893 a.u.

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:    -117.92196  -12.28630   -9.53294   -9.53294   -9.53294

                        A         A         A         A         A
   1 Ar  1 S         0.98406    0.30614    0.00000    0.00000    0.00000
   2 Ar  1 S         0.07605   -0.92385    0.00000    0.00000    0.00000
   3 Ar  1 PX        0.00000    0.00000   -0.91582   -0.04209   -0.33196
   4 Ar  1 PY        0.00000    0.00000    0.26552   -0.68007   -0.64629
   5 Ar  1 PZ        0.00000    0.00000   -0.20363   -0.69744    0.65023
   6 Ar  1 S        -0.08062   -0.29753    0.00000    0.00000    0.00000
   7 Ar  1 PX        0.00000    0.00000   -0.07056   -0.00324   -0.02558
   8 Ar  1 PY        0.00000    0.00000    0.02046   -0.05240   -0.04980
   9 Ar  1 PZ        0.00000    0.00000   -0.01569   -0.05374    0.05010
  10 Ar  1 S        -0.00718    0.00786    0.00000    0.00000    0.00000
  11 Ar  1 PX        0.00000    0.00000    0.02008    0.00092    0.00728
  12 Ar  1 PY        0.00000    0.00000   -0.00582    0.01491    0.01417
  13 Ar  1 PZ        0.00000    0.00000    0.00446    0.01529   -0.01426
  14 Ar  1 DXX       0.03186    0.08243    0.00000    0.00000    0.00000
  15 Ar  1 DYY       0.03186    0.08243    0.00000    0.00000    0.00000
  16 Ar  1 DZZ       0.03186    0.08243    0.00000    0.00000    0.00000
  17 Ar  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 Ar  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 Ar  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:			6	7	8	9	10
Eigenvalues:			-1.27172	-0.58870	-0.58870	-0.58870	0.69268
			A	A	A	A	A
1	Ar	1 S	-0.08365	0.00000	0.00000	0.00000	0.05849
2	Ar	1 S	0.48696	0.00000	0.00000	0.00000	-0.29851
3	Ar	1 PX	0.00000	-0.11552	0.11153	-0.25288	0.00000
4	Ar	1 PY	0.00000	-0.19694	-0.22552	-0.00950	0.00000
5	Ar	1 PZ	0.00000	0.19392	-0.16259	-0.16029	0.00000
6	Ar	1 S	-0.60726	0.00000	0.00000	0.00000	1.40310
7	Ar	1 PX	0.00000	0.25658	-0.24772	0.56166	0.00000
8	Ar	1 PY	0.00000	0.43741	0.50089	0.02110	0.00000
9	Ar	1 PZ	0.00000	-0.43070	0.36112	0.35602	0.00000
10	Ar	1 S	-0.45332	0.00000	0.00000	0.00000	-1.85205
11	Ar	1 PX	0.00000	0.18341	-0.17708	0.40150	0.00000
12	Ar	1 PY	0.00000	0.31268	0.35805	0.01508	0.00000
13	Ar	1 PZ	0.00000	-0.30788	0.25814	0.25450	0.00000
14	Ar	1 DXX	-0.02921	0.00000	0.00000	0.00000	0.22214
15	Ar	1 DYY	-0.02921	0.00000	0.00000	0.00000	0.22214
16	Ar	1 DZZ	-0.02921	0.00000	0.00000	0.00000	0.22214
17	Ar	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Ar	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Ar	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:			11	12	13	14	15
Eigenvalues:			0.86565	0.86565	0.86565	1.21161	1.21161
			A	A	A	A	A
1	Ar	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2	Ar	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3	Ar	1 PX	-0.06850	0.01049	-0.33673	0.00000	0.00000
4	Ar	1 PY	-0.23562	0.24411	0.05554	0.00000	0.00000
5	Ar	1 PZ	0.24079	0.24185	-0.04145	0.00000	0.00000
6	Ar	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7	Ar	1 PX	0.23787	-0.03644	1.16926	0.00000	0.00000
8	Ar	1 PY	0.81816	-0.84764	-0.19286	0.00000	0.00000
9	Ar	1 PZ	-0.83612	-0.83980	0.14392	0.00000	0.00000
10	Ar	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11	Ar	1 PX	-0.24017	0.03679	-1.18056	0.00000	0.00000
12	Ar	1 PY	-0.82607	0.85583	0.19472	0.00000	0.00000
13	Ar	1 PZ	0.84420	0.84791	-0.14531	0.00000	0.00000
14	Ar	1 DXX	0.00000	0.00000	0.00000	0.09490	0.99456
15	Ar	1 DYY	0.00000	0.00000	0.00000	0.79864	-0.58035
16	Ar	1 DZZ	0.00000	0.00000	0.00000	-0.89353	-0.41421
17	Ar	1 DXY	0.00000	0.00000	0.00000	0.13932	0.01413
18	Ar	1 DXZ	0.00000	0.00000	0.00000	0.13062	-0.01850
19	Ar	1 DYZ	0.00000	0.00000	0.00000	-0.00658	0.03313

MO:			16	17	18	19
Eigenvalues:			1.21161	1.21161	1.21161	4.68648
			A	A	A	A
1	Ar	1 S	0.00000	0.00000	0.00000	-0.11998
2	Ar	1 S	0.00000	0.00000	0.00000	1.53523
3	Ar	1 PX	0.00000	0.00000	0.00000	0.00000
4	Ar	1 PY	0.00000	0.00000	0.00000	0.00000
5	Ar	1 PZ	0.00000	0.00000	0.00000	0.00000

```
   6 Ar   1 S          0.00000    0.00000    0.00000   -4.36488
   7 Ar   1 PX         0.00000    0.00000    0.00000    0.00000
   8 Ar   1 PY         0.00000    0.00000    0.00000    0.00000
   9 Ar   1 PZ         0.00000    0.00000    0.00000    0.00000
  10 Ar   1 S          0.00000    0.00000    0.00000   -0.86197
  11 Ar   1 PX         0.00000    0.00000    0.00000    0.00000
  12 Ar   1 PY         0.00000    0.00000    0.00000    0.00000
  13 Ar   1 PZ         0.00000    0.00000    0.00000    0.00000
  14 Ar   1 DXX       -0.00233   -0.02429    0.03521    2.11803
  15 Ar   1 DYY        0.02268    0.10721    0.11557    2.11803
  16 Ar   1 DZZ       -0.02035   -0.08292   -0.15079    2.11803
  17 Ar   1 DXY       -0.58602    0.02268   -0.79778    0.00000
  18 Ar   1 DXZ        0.47404   -0.79780   -0.34841    0.00000
  19 Ar   1 DYZ        0.65669    0.59191   -0.46612    0.00000

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  1.77 secs.
  Total Wall time:       0 mins.  2.32 secs.

  Calculation finished: Fri Sep 18 13:39:37 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.04 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:30:25 1998

  Run type: Single point energy
  Model: RHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  10
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Na Na1          0.0000000     2.7751482    -1.7280983

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  RHF direct SCF procedure requested

  Energy converged to -.11E-09 in   7 cycles

  E(HF)  =    -160.6747427 a.u.

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -40.50202   -3.04847   -1.76732   -1.76732   -1.76732

                        A         A         A         A         A
   1 Na  1 S         0.99047    0.26882    0.00000    0.00000    0.00000
   2 Na  1 S         0.03881   -1.02133    0.00000    0.00000    0.00000
   3 Na  1 PX        0.00000    0.00000   -0.41484   -0.01583   -0.90155
   4 Na  1 PY        0.00000    0.00000   -0.46510    0.85393    0.19902
   5 Na  1 PZ        0.00000    0.00000   -0.77248   -0.50565    0.36432
   6 Na  1 S        -0.00650    0.04284    0.00000    0.00000    0.00000
   7 Na  1 PX        0.00000    0.00000   -0.02700   -0.00103   -0.05867
   8 Na  1 PY        0.00000    0.00000   -0.03027    0.05557    0.01295
   9 Na  1 PZ        0.00000    0.00000   -0.05027   -0.03291    0.02371
  10 Na  1 S         0.00211   -0.00685    0.00000    0.00000    0.00000
  11 Na  1 PX        0.00000    0.00000    0.01364    0.00052    0.02964
  12 Na  1 PY        0.00000    0.00000    0.01529   -0.02807   -0.00654
  13 Na  1 PZ        0.00000    0.00000    0.02540    0.01662   -0.01198
  14 Na  1 DXX       0.00017   -0.02919    0.00000    0.00000    0.00000
  15 Na  1 DYY       0.00017   -0.02919    0.00000    0.00000    0.00000
  16 Na  1 DZZ       0.00017   -0.02919    0.00000    0.00000    0.00000
  17 Na  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 Na  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 Na  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:		6	7	8	9	10
Eigenvalues:		-0.18013	-0.10866	-0.10866	-0.10866	-0.03513
		A	A	A	A	A
1	Na 1 S	0.03841	0.00000	0.00000	0.00000	-0.02601
2	Na 1 S	-0.18999	0.00000	0.00000	0.00000	-0.04806
3	Na 1 PX	0.00000	-0.08626	0.03410	-0.03705	0.00000
4	Na 1 PY	0.00000	-0.02880	-0.09370	-0.01919	0.00000
5	Na 1 PZ	0.00000	-0.04131	-0.00589	0.09075	0.00000
6	Na 1 S	0.53235	0.00000	0.00000	0.00000	-3.26719
7	Na 1 PX	0.00000	0.33272	-0.13153	0.14291	0.00000
8	Na 1 PY	0.00000	0.11107	0.36140	0.07403	0.00000
9	Na 1 PZ	0.00000	0.15933	0.02273	-0.35003	0.00000
10	Na 1 S	0.52308	0.00000	0.00000	0.00000	2.43990
11	Na 1 PX	0.00000	0.58168	-0.22995	0.24985	0.00000
12	Na 1 PY	0.00000	0.19418	0.63182	0.12942	0.00000
13	Na 1 PZ	0.00000	0.27856	0.03974	-0.61195	0.00000
14	Na 1 DXX	-0.00467	0.00000	0.00000	0.00000	0.41890
15	Na 1 DYY	-0.00467	0.00000	0.00000	0.00000	0.41890
16	Na 1 DZZ	-0.00467	0.00000	0.00000	0.00000	0.41890
17	Na 1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Na 1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Na 1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		-0.00035	-0.00035	-0.00035	0.24136	0.24136
		A	A	A	A	A
1	Na 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2	Na 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3	Na 1 PX	0.11287	-0.00207	-0.12044	0.00000	0.00000
4	Na 1 PY	0.06254	0.14208	0.05616	0.00000	0.00000
5	Na 1 PZ	0.10296	-0.08402	0.09793	0.00000	0.00000
6	Na 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7	Na 1 PX	-1.06163	0.01950	1.13290	0.00000	0.00000
8	Na 1 PY	-0.58822	-1.33638	-0.52821	0.00000	0.00000
9	Na 1 PZ	-0.96842	0.79034	-0.92111	0.00000	0.00000
10	Na 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11	Na 1 PX	0.98500	-0.01809	-1.05112	0.00000	0.00000
12	Na 1 PY	0.54576	1.23991	0.49008	0.00000	0.00000
13	Na 1 PZ	0.89852	-0.73329	0.85461	0.00000	0.00000
14	Na 1 DXX	0.00000	0.00000	0.00000	-0.12813	0.80172
15	Na 1 DYY	0.00000	0.00000	0.00000	-0.66425	-0.54073
16	Na 1 DZZ	0.00000	0.00000	0.00000	0.79238	-0.26098
17	Na 1 DXY	0.00000	0.00000	0.00000	0.26905	0.44205
18	Na 1 DXZ	0.00000	0.00000	0.00000	0.25018	-0.31113
19	Na 1 DYZ	0.00000	0.00000	0.00000	0.37597	-0.19736

MO:		16	17	18	19
Eigenvalues:		0.24136	0.24136	0.24136	0.34401
		A	A	A	A
1	Na 1 S	0.00000	0.00000	0.00000	-0.00100
2	Na 1 S	0.00000	0.00000	0.00000	0.12244
3	Na 1 PX	0.00000	0.00000	0.00000	0.00000
4	Na 1 PY	0.00000	0.00000	0.00000	0.00000
5	Na 1 PZ	0.00000	0.00000	0.00000	0.00000

```
   6 Na   1 S          0.00000    0.00000    0.00000    6.72306
   7 Na   1 PX         0.00000    0.00000    0.00000    0.00000
   8 Na   1 PY         0.00000    0.00000    0.00000    0.00000
   9 Na   1 PZ         0.00000    0.00000    0.00000    0.00000
  10 Na   1 S          0.00000    0.00000    0.00000   -2.15627
  11 Na   1 PX         0.00000    0.00000    0.00000    0.00000
  12 Na   1 PY         0.00000    0.00000    0.00000    0.00000
  13 Na   1 PZ         0.00000    0.00000    0.00000    0.00000
  14 Na   1 DXX        0.13985    0.37152    0.42808   -2.29769
  15 Na   1 DYY       -0.02993    0.16548   -0.48796   -2.29769
  16 Na   1 DZZ       -0.10992   -0.53699    0.05988   -2.29769
  17 Na   1 DXY       -0.30426    0.15700   -0.78421    0.00000
  18 Na   1 DXZ       -0.57063    0.66677    0.26533    0.00000
  19 Na   1 DYZ        0.74841    0.47776   -0.17699    0.00000

    ** Archive file written to unit 12 **

  Total Cpu time:         0 mins.  1.11 secs.
  Total Wall time:        0 mins.  1.48 secs.

  Calculation finished: Fri Sep 18 13:30:26 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.04 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:31:43 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  11
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Mg Mg1          0.0000002     1.2011840     2.6260351

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.11E-06 in   6 cycles  <S**2> = 0.7500

  E(HF)  =    -198.2425123 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -49.02809   -4.06751   -2.57480   -2.57480   -2.57480

                        A         A         A         A         A
   1 Mg  1 S         0.98873    0.27488    0.00000    0.00000    0.00000
   2 Mg  1 S         0.04677   -1.00085    0.00000    0.00000    0.00000
   3 Mg  1 PX        0.00000    0.00000   -0.44394   -0.13260    0.86552
   4 Mg  1 PY        0.00000    0.00000   -0.67548    0.66934   -0.24393
   5 Mg  1 PZ        0.00000    0.00000   -0.55716   -0.70583   -0.39391
   6 Mg  1 S        -0.03291   -0.14550    0.00000    0.00000    0.00000
   7 Mg  1 PX        0.00000    0.00000   -0.03913   -0.01169    0.07629
   8 Mg  1 PY        0.00000    0.00000   -0.05954    0.05900   -0.02150
   9 Mg  1 PZ        0.00000    0.00000   -0.04911   -0.06221   -0.03472
  10 Mg  1 S        -0.01232   -0.01468    0.00000    0.00000    0.00000
  11 Mg  1 PX        0.00000    0.00000    0.01441    0.00430   -0.02810
  12 Mg  1 PY        0.00000    0.00000    0.02193   -0.02173    0.00792
  13 Mg  1 PZ        0.00000    0.00000    0.01809    0.02291    0.01279
  14 Mg  1 DXX       0.01728    0.05107    0.00000    0.00000    0.00000
  15 Mg  1 DYY       0.01728    0.05107    0.00000    0.00000    0.00000
  16 Mg  1 DZZ       0.01728    0.05107    0.00000    0.00000    0.00000
  17 Mg  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 Mg  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 Mg  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:		6	7	8	9	10
Eigenvalues:		-0.53793	-0.17119	-0.17119	-0.17119	0.02047
		A	A	A	A	A
1	Mg 1 S	-0.05606	0.00000	0.00000	0.00000	-0.02929
2	Mg 1 S	0.27193	0.00000	0.00000	0.00000	-0.01706
3	Mg 1 PX	0.00000	0.04702	-0.03350	-0.15657	0.00000
4	Mg 1 PY	0.00000	0.12658	0.10772	0.01497	0.00000
5	Mg 1 PZ	0.00000	0.09806	-0.12298	0.05576	0.00000
6	Mg 1 S	-0.61590	0.00000	0.00000	0.00000	-1.51333
7	Mg 1 PX	0.00000	-0.11768	0.08384	0.39184	0.00000
8	Mg 1 PY	0.00000	-0.31678	-0.26957	-0.03746	0.00000
9	Mg 1 PZ	0.00000	-0.24540	0.30777	-0.13956	0.00000
10	Mg 1 S	-0.40877	0.00000	0.00000	0.00000	1.92237
11	Mg 1 PX	0.00000	-0.18976	0.13520	0.63184	0.00000
12	Mg 1 PY	0.00000	-0.51079	-0.43468	-0.06040	0.00000
13	Mg 1 PZ	0.00000	-0.39571	0.49627	-0.22503	0.00000
14	Mg 1 DXX	-0.01829	0.00000	0.00000	0.00000	-0.15016
15	Mg 1 DYY	-0.01829	0.00000	0.00000	0.00000	-0.15016
16	Mg 1 DZZ	-0.01829	0.00000	0.00000	0.00000	-0.15016
17	Mg 1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Mg 1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Mg 1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.07970	0.07970	0.07970	0.16154	0.16154
		A	A	A	A	A
1	Mg 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2	Mg 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3	Mg 1 PX	0.12839	-0.03478	-0.22391	0.00000	0.00000
4	Mg 1 PY	0.17513	0.17853	0.07269	0.00000	0.00000
5	Mg 1 PZ	0.14378	-0.18640	0.11140	0.00000	0.00000
6	Mg 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7	Mg 1 PX	-0.66296	0.17961	1.15622	0.00000	0.00000
8	Mg 1 PY	-0.90435	-0.92191	-0.37534	0.00000	0.00000
9	Mg 1 PZ	-0.74247	0.96253	-0.57524	0.00000	0.00000
10	Mg 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11	Mg 1 PX	0.59516	-0.16124	-1.03798	0.00000	0.00000
12	Mg 1 PY	0.81186	0.82762	0.33695	0.00000	0.00000
13	Mg 1 PZ	0.66654	-0.86409	0.51641	0.00000	0.00000
14	Mg 1 DXX	0.00000	0.00000	0.00000	-0.26384	0.93696
15	Mg 1 DYY	0.00000	0.00000	0.00000	-0.68587	-0.71368
16	Mg 1 DZZ	0.00000	0.00000	0.00000	0.94971	-0.22327
17	Mg 1 DXY	0.00000	0.00000	0.00000	0.02984	-0.11997
18	Mg 1 DXZ	0.00000	0.00000	0.00000	-0.03750	-0.12329
19	Mg 1 DYZ	0.00000	0.00000	0.00000	-0.19073	0.11115

MO:		16	17	18	19
Eigenvalues:		0.16154	0.16154	0.16154	0.66047
		A	A	A	A
1	Mg 1 S	0.00000	0.00000	0.00000	-0.09353
2	Mg 1 S	0.00000	0.00000	0.00000	0.57444
3	Mg 1 PX	0.00000	0.00000	0.00000	0.00000
4	Mg 1 PY	0.00000	0.00000	0.00000	0.00000
5	Mg 1 PZ	0.00000	0.00000	0.00000	0.00000

6	Mg	1	S	0.00000	0.00000	0.00000	-2.67074
7	Mg	1	PX	0.00000	0.00000	0.00000	0.00000
8	Mg	1	PY	0.00000	0.00000	0.00000	0.00000
9	Mg	1	PZ	0.00000	0.00000	0.00000	0.00000
10	Mg	1	S	0.00000	0.00000	0.00000	-1.41988
11	Mg	1	PX	0.00000	0.00000	0.00000	0.00000
12	Mg	1	PY	0.00000	0.00000	0.00000	0.00000
13	Mg	1	PZ	0.00000	0.00000	0.00000	0.00000
14	Mg	1	DXX	0.09029	0.03265	0.20804	1.77643
15	Mg	1	DYY	0.09567	0.01921	-0.10354	1.77643
16	Mg	1	DZZ	-0.18596	-0.05186	-0.10451	1.77643
17	Mg	1	DXY	-0.23603	0.78652	0.55713	0.00000
18	Mg	1	DXZ	-0.27967	-0.61532	0.72565	0.00000
19	Mg	1	DYZ	-0.91186	-0.00432	-0.34607	0.00000

Beta Spin Molecular Orbital Coefficients

MO:				1	2	3	4	5
Eigenvalues:				-49.02216	-4.05260	-2.56969	-2.56969	-2.56969
				A	A	A	A	A
1	Mg	1	S	-0.98871	-0.27470	0.00000	0.00000	0.00000
2	Mg	1	S	-0.04684	0.99962	0.00000	0.00000	0.00000
3	Mg	1	PX	0.00000	0.00000	-0.78815	-0.13169	-0.57223
4	Mg	1	PY	0.00000	0.00000	-0.48879	0.67790	0.51721
5	Mg	1	PZ	0.00000	0.00000	-0.32539	-0.69934	0.60911
6	Mg	1	S	0.03296	0.15132	0.00000	0.00000	0.00000
7	Mg	1	PX	0.00000	0.00000	-0.06589	-0.01101	-0.04784
8	Mg	1	PY	0.00000	0.00000	-0.04086	0.05667	0.04324
9	Mg	1	PZ	0.00000	0.00000	-0.02720	-0.05847	0.05092
10	Mg	1	S	0.01235	0.01638	0.00000	0.00000	0.00000
11	Mg	1	PX	0.00000	0.00000	0.02509	0.00419	0.01821
12	Mg	1	PY	0.00000	0.00000	0.01556	-0.02158	-0.01646
13	Mg	1	PZ	0.00000	0.00000	0.01036	0.02226	-0.01939
14	Mg	1	DXX	-0.01731	-0.05380	0.00000	0.00000	0.00000
15	Mg	1	DYY	-0.01731	-0.05380	0.00000	0.00000	0.00000
16	Mg	1	DZZ	-0.01731	-0.05380	0.00000	0.00000	0.00000
17	Mg	1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Mg	1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Mg	1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:				6	7	8	9	10
Eigenvalues:				-0.23553	-0.12418	-0.12418	-0.12418	0.05351
				A	A	A	A	A
1	Mg	1	S	0.04756	0.00000	0.00000	0.00000	-0.03615
2	Mg	1	S	-0.25716	0.00000	0.00000	0.00000	0.01462
3	Mg	1	PX	0.00000	0.07319	0.02455	0.10107	0.00000
4	Mg	1	PY	0.00000	0.08666	-0.08273	-0.04266	0.00000
5	Mg	1	PZ	0.00000	0.05751	0.09342	-0.06434	0.00000
6	Mg	1	S	0.25564	0.00000	0.00000	0.00000	-1.50744
7	Mg	1	PX	0.00000	-0.13317	-0.04466	-0.18390	0.00000
8	Mg	1	PY	0.00000	-0.15768	0.15053	0.07762	0.00000
9	Mg	1	PZ	0.00000	-0.10465	-0.16998	0.11706	0.00000
10	Mg	1	S	0.72671	0.00000	0.00000	0.00000	1.86080
11	Mg	1	PX	0.00000	-0.47824	-0.16040	-0.66043	0.00000
12	Mg	1	PY	0.00000	-0.56627	0.54060	0.27876	0.00000
13	Mg	1	PZ	0.00000	-0.37582	-0.61044	0.42040	0.00000
14	Mg	1	DXX	0.03346	0.00000	0.00000	0.00000	-0.21284

15 Mg	1 DYY	0.03346	0.00000	0.00000	0.00000	-0.21284
16 Mg	1 DZZ	0.03346	0.00000	0.00000	0.00000	-0.21284
17 Mg	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18 Mg	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 Mg	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.11248	0.11248	0.11248	0.19449	0.19449
		A	A	A	A	A
1 Mg	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 Mg	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 Mg	1 PX	0.16220	-0.00206	-0.22585	0.00000	0.00000
4 Mg	1 PY	0.12555	0.23196	0.08805	0.00000	0.00000
5 Mg	1 PZ	0.18775	-0.15334	0.13623	0.00000	0.00000
6 Mg	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 Mg	1 PX	-0.81041	0.01030	1.12844	0.00000	0.00000
8 Mg	1 PY	-0.62732	-1.15895	-0.43994	0.00000	0.00000
9 Mg	1 PZ	-0.93805	0.76614	-0.68068	0.00000	0.00000
10 Mg	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 Mg	1 PX	0.64443	-0.00819	-0.89732	0.00000	0.00000
12 Mg	1 PY	0.49884	0.92158	0.34984	0.00000	0.00000
13 Mg	1 PZ	0.74593	-0.60923	0.54127	0.00000	0.00000
14 Mg	1 DXX	0.00000	0.00000	0.00000	0.82700	-0.42303
15 Mg	1 DYY	0.00000	0.00000	0.00000	-0.05592	0.92275
16 Mg	1 DZZ	0.00000	0.00000	0.00000	-0.77108	-0.49972
17 Mg	1 DXY	0.00000	0.00000	0.00000	0.26073	-0.05222
18 Mg	1 DXZ	0.00000	0.00000	0.00000	-0.21681	0.16364
19 Mg	1 DYZ	0.00000	0.00000	0.00000	-0.17491	-0.34214

MO:		16	17	18	19
Eigenvalues:		0.19449	0.19449	0.19449	0.68868
		A	A	A	A
1 Mg	1 S	0.00000	0.00000	0.00000	-0.09650
2 Mg	1 S	0.00000	0.00000	0.00000	0.58338
3 Mg	1 PX	0.00000	0.00000	0.00000	0.00000
4 Mg	1 PY	0.00000	0.00000	0.00000	0.00000
5 Mg	1 PZ	0.00000	0.00000	0.00000	0.00000
6 Mg	1 S	0.00000	0.00000	0.00000	-2.73184
7 Mg	1 PX	0.00000	0.00000	0.00000	0.00000
8 Mg	1 PY	0.00000	0.00000	0.00000	0.00000
9 Mg	1 PZ	0.00000	0.00000	0.00000	0.00000
10 Mg	1 S	0.00000	0.00000	0.00000	-1.37403
11 Mg	1 PX	0.00000	0.00000	0.00000	0.00000
12 Mg	1 PY	0.00000	0.00000	0.00000	0.00000
13 Mg	1 PZ	0.00000	0.00000	0.00000	0.00000
14 Mg	1 DXX	-0.04269	0.17924	0.32119	1.76971
15 Mg	1 DYY	0.15944	-0.34596	0.01687	1.76971
16 Mg	1 DZZ	-0.11675	0.16672	-0.33806	1.76971
17 Mg	1 DXY	0.65575	0.08658	-0.70128	0.00000
18 Mg	1 DXZ	0.47537	0.71202	0.43961	0.00000
19 Mg	1 DYZ	0.56283	-0.60480	0.41206	0.00000

** Archive file written to unit 12 **

Total Cpu time: 0 mins. 1.30 secs.
Total Wall time: 0 mins. 2.39 secs.

```
  Calculation finished: Fri Sep 18 13:31:45 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:33:05 1998

  Run type: Single point energy
  Model: RHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  12
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Al Al1         -0.0000001     0.0000000    -1.1017752

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  RHF direct SCF procedure requested

  Energy converged to -.24E-05 in   5 cycles

  E(HF)  =    -240.3814048 a.u.

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -58.44404   -5.19389   -3.49460   -3.49460   -3.49460

                        A         A         A         A         A
   1 Al  1 S        -0.98703   -0.28069    0.00000    0.00000    0.00000
   2 Al  1 S        -0.05412    0.98968    0.00000    0.00000    0.00000
   3 Al  1 PX        0.00000    0.00000    0.94708   -0.15217    0.19998
   4 Al  1 PY        0.00000    0.00000   -0.11036   -0.95242   -0.20205
   5 Al  1 PZ        0.00000    0.00000   -0.22576   -0.17276    0.93771
   6 Al  1 S         0.09443    0.26726    0.00000    0.00000    0.00000
   7 Al  1 PX        0.00000    0.00000    0.07900   -0.01269    0.01668
   8 Al  1 PY        0.00000    0.00000   -0.00921   -0.07945   -0.01685
   9 Al  1 PZ        0.00000    0.00000   -0.01883   -0.01441    0.07822
  10 Al  1 S         0.00003   -0.02454    0.00000    0.00000    0.00000
  11 Al  1 PX        0.00000    0.00000   -0.02720    0.00437   -0.00574
  12 Al  1 PY        0.00000    0.00000    0.00317    0.02735    0.00580
  13 Al  1 PZ        0.00000    0.00000    0.00648    0.00496   -0.02693
  14 Al  1 DXX      -0.03861   -0.08372    0.00000    0.00000    0.00000
  15 Al  1 DYY      -0.03861   -0.08372    0.00000    0.00000    0.00000
  16 Al  1 DZZ      -0.03861   -0.08372    0.00000    0.00000    0.00000
  17 Al  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 Al  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 Al  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:			6	7	8	9	10
Eigenvalues:			-0.64962	-0.19594	-0.19594	-0.19594	0.06916
			A	A	A	A	A
1	Al	1 S	0.06486	0.00000	0.00000	0.00000	0.05032
2	Al	1 S	-0.31397	0.00000	0.00000	0.00000	-0.08618
3	Al	1 PX	0.00000	0.13474	0.07767	-0.09949	0.00000
4	Al	1 PY	0.00000	0.06838	-0.16724	-0.03795	0.00000
5	Al	1 PZ	0.00000	-0.10609	-0.00915	-0.15082	0.00000
6	Al	1 S	0.57001	0.00000	0.00000	0.00000	1.57391
7	Al	1 PX	0.00000	-0.31093	-0.17922	0.22959	0.00000
8	Al	1 PY	0.00000	-0.15779	0.38593	0.08758	0.00000
9	Al	1 PZ	0.00000	0.24482	0.02111	0.34803	0.00000
10	Al	1 S	0.46146	0.00000	0.00000	0.00000	-1.71697
11	Al	1 PX	0.00000	-0.49240	-0.28383	0.36359	0.00000
12	Al	1 PY	0.00000	-0.24988	0.61118	0.13870	0.00000
13	Al	1 PZ	0.00000	0.38771	0.03343	0.55116	0.00000
14	Al	1 DXX	0.02122	0.00000	0.00000	0.00000	0.04919
15	Al	1 DYY	0.02122	0.00000	0.00000	0.00000	0.04919
16	Al	1 DZZ	0.02122	0.00000	0.00000	0.00000	0.04919
17	Al	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Al	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Al	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:			11	12	13	14	15
Eigenvalues:			0.14168	0.14168	0.14168	0.38552	0.38552
			A	A	A	A	A
1	Al	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2	Al	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3	Al	1 PX	-0.14676	-0.22171	-0.13580	0.00000	0.00000
4	Al	1 PY	-0.18820	0.19818	-0.12017	0.00000	0.00000
5	Al	1 PZ	0.17939	0.02653	-0.23717	0.00000	0.00000
6	Al	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7	Al	1 PX	0.64908	0.98060	0.60062	0.00000	0.00000
8	Al	1 PY	0.83236	-0.87652	0.53151	0.00000	0.00000
9	Al	1 PZ	-0.79340	-0.11734	1.04898	0.00000	0.00000
10	Al	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11	Al	1 PX	-0.57520	-0.86898	-0.53226	0.00000	0.00000
12	Al	1 PY	-0.73762	0.77675	-0.47101	0.00000	0.00000
13	Al	1 PZ	0.70309	0.10399	-0.92958	0.00000	0.00000
14	Al	1 DXX	0.00000	0.00000	0.00000	0.90423	-0.10814
15	Al	1 DYY	0.00000	0.00000	0.00000	-0.51036	0.61855
16	Al	1 DZZ	0.00000	0.00000	0.00000	-0.39387	-0.51041
17	Al	1 DXY	0.00000	0.00000	0.00000	0.05835	0.63840
18	Al	1 DXZ	0.00000	0.00000	0.00000	0.41500	0.28274
19	Al	1 DYZ	0.00000	0.00000	0.00000	-0.04705	0.27559

MO:			16	17	18	19
Eigenvalues:			0.38552	0.38552	0.38552	1.65984
			A	A	A	A
1	Al	1 S	0.00000	0.00000	0.00000	-0.13127
2	Al	1 S	0.00000	0.00000	0.00000	0.78911
3	Al	1 PX	0.00000	0.00000	0.00000	0.00000
4	Al	1 PY	0.00000	0.00000	0.00000	0.00000
5	Al	1 PZ	0.00000	0.00000	0.00000	0.00000

```
   6 Al  1 S         0.00000    0.00000    0.00000   -6.18187
   7 Al  1 PX        0.00000    0.00000    0.00000    0.00000
   8 Al  1 PY        0.00000    0.00000    0.00000    0.00000
   9 Al  1 PZ        0.00000    0.00000    0.00000    0.00000
  10 Al  1 S         0.00000    0.00000    0.00000   -0.30983
  11 Al  1 PX        0.00000    0.00000    0.00000    0.00000
  12 Al  1 PY        0.00000    0.00000    0.00000    0.00000
  13 Al  1 PZ        0.00000    0.00000    0.00000    0.00000
  14 Al  1 DXX       0.31849   -0.00603    0.26306    2.84320
  15 Al  1 DYY       0.10752    0.58761   -0.00883    2.84320
  16 Al  1 DZZ      -0.42601   -0.58158   -0.25422    2.84320
  17 Al  1 DXY       0.25760   -0.67246   -0.26546    0.00000
  18 Al  1 DXZ      -0.73128    0.19030   -0.42053    0.00000
  19 Al  1 DYZ      -0.45005   -0.23638    0.81450    0.00000

    ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  1.10 secs.
  Total Wall time:       0 mins.  1.65 secs.

  Calculation finished: Fri Sep 18 13:33:06 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.05 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:34:27 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  13
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Si Si1          0.0000001     2.3195269    -0.9577252

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.15E-06 in   6 cycles  <S**2> = 0.7581

  E(HF)  =    -287.1123169 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -68.76201   -6.49614   -4.60004   -4.58776   -4.58776

                        A         A         A         A         A
   1 Si  1 S         0.98615    0.28632    0.00000    0.00000    0.00000
   2 Si  1 S         0.06086   -0.97189    0.00000    0.00000    0.00000
   3 Si  1 PX        0.00000    0.00000    0.97696    0.00000    0.00000
   4 Si  1 PY        0.00000    0.00000    0.00000   -0.93050   -0.29275
   5 Si  1 PZ        0.00000    0.00000    0.00000   -0.29275    0.93050
   6 Si  1 S        -0.10297   -0.30581    0.00000    0.00000    0.00000
   7 Si  1 PX        0.00000    0.00000    0.08067    0.00000    0.00000
   8 Si  1 PY        0.00000    0.00000    0.00000   -0.08165   -0.02569
   9 Si  1 PZ        0.00000    0.00000    0.00000   -0.02569    0.08165
  10 Si  1 S        -0.00350    0.01825    0.00000    0.00000    0.00000
  11 Si  1 PX        0.00000    0.00000   -0.02425    0.00000    0.00000
  12 Si  1 PY        0.00000    0.00000    0.00000    0.02502    0.00787
  13 Si  1 PZ        0.00000    0.00000    0.00000    0.00787   -0.02502
  14 Si  1 DXX       0.04269    0.09596    0.00000    0.00000    0.00000
  15 Si  1 DYY       0.04272    0.09613    0.00000    0.00000    0.00000
  16 Si  1 DZZ       0.04272    0.09613    0.00000    0.00000    0.00000
  17 Si  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 Si  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 Si  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:		6	7	8	9	10
Eigenvalues:		-0.88154	-0.59343	-0.26607	-0.26607	0.14771
		A	A	A	A	A
1	Si 1 S	-0.07093	0.00000	0.00000	0.00000	0.05750
2	Si 1 S	0.35941	0.00000	0.00000	0.00000	-0.13894
3	Si 1 PX	0.00000	-0.26035	0.00000	0.00000	0.00000
4	Si 1 PY	0.00000	0.00000	0.20312	-0.07799	0.00000
5	Si 1 PZ	0.00000	0.00000	0.07799	0.20312	0.00000
6	Si 1 S	-0.49313	0.00000	0.00000	0.00000	1.56211
7	Si 1 PX	0.00000	0.62693	0.00000	0.00000	0.00000
8	Si 1 PY	0.00000	0.00000	-0.41723	0.16020	0.00000
9	Si 1 PZ	0.00000	0.00000	-0.16020	-0.41723	0.00000
10	Si 1 S	-0.51668	0.00000	0.00000	0.00000	-1.72847
11	Si 1 PX	0.00000	0.49501	0.00000	0.00000	0.00000
12	Si 1 PY	0.00000	0.00000	-0.62019	0.23813	0.00000
13	Si 1 PZ	0.00000	0.00000	-0.23813	-0.62019	0.00000
14	Si 1 DXX	-0.08125	0.00000	0.00000	0.00000	0.08476
15	Si 1 DYY	-0.01103	0.00000	0.00000	0.00000	0.07898
16	Si 1 DZZ	-0.01103	0.00000	0.00000	0.00000	0.07898
17	Si 1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Si 1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Si 1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.21046	0.24196	0.24196	0.45510	0.46104
		A	A	A	A	A
1	Si 1 S	0.00000	0.00000	0.00000	-0.00360	0.00000
2	Si 1 S	0.00000	0.00000	0.00000	0.01813	0.00000
3	Si 1 PX	0.30072	0.00000	0.00000	0.00000	0.00000
4	Si 1 PY	0.00000	-0.33064	0.06681	0.00000	0.00000
5	Si 1 PZ	0.00000	-0.06681	-0.33064	0.00000	0.00000
6	Si 1 S	0.00000	0.00000	0.00000	-0.03438	0.00000
7	Si 1 PX	-1.23225	0.00000	0.00000	0.00000	0.00000
8	Si 1 PY	0.00000	1.28211	-0.25906	0.00000	0.00000
9	Si 1 PZ	0.00000	0.25906	1.28211	0.00000	0.00000
10	Si 1 S	0.00000	0.00000	0.00000	-0.01801	0.00000
11	Si 1 PX	1.23676	0.00000	0.00000	0.00000	0.00000
12	Si 1 PY	0.00000	-1.13176	0.22868	0.00000	0.00000
13	Si 1 PZ	0.00000	-0.22868	-1.13176	0.00000	0.00000
14	Si 1 DXX	0.00000	0.00000	0.00000	0.99942	0.00000
15	Si 1 DYY	0.00000	0.00000	0.00000	-0.49892	0.00000
16	Si 1 DZZ	0.00000	0.00000	0.00000	-0.49892	0.00000
17	Si 1 DXY	0.00000	0.00000	0.00000	0.00000	-0.98247
18	Si 1 DXZ	0.00000	0.00000	0.00000	0.00000	-0.18643
19	Si 1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		16	17	18	19
Eigenvalues:		0.46104	0.48474	0.48474	2.22951
		A	A	A	A
1	Si 1 S	0.00000	0.00000	0.00000	-0.13130
2	Si 1 S	0.00000	0.00000	0.00000	1.04895
3	Si 1 PX	0.00000	0.00000	0.00000	0.00000
4	Si 1 PY	0.00000	0.00000	0.00000	0.00000
5	Si 1 PZ	0.00000	0.00000	0.00000	0.00000

6	Si	1	S	0.00000	0.00000	0.00000	-6.32798
7	Si	1	PX	0.00000	0.00000	0.00000	0.00000
8	Si	1	PY	0.00000	0.00000	0.00000	0.00000
9	Si	1	PZ	0.00000	0.00000	0.00000	0.00000
10	Si	1	S	0.00000	0.00000	0.00000	-0.56695
11	Si	1	PX	0.00000	0.00000	0.00000	0.00000
12	Si	1	PY	0.00000	0.00000	0.00000	0.00000
13	Si	1	PZ	0.00000	0.00000	0.00000	0.00000
14	Si	1	DXX	0.00000	0.00000	0.00000	2.96325
15	Si	1	DYY	0.00000	-0.86503	-0.04154	2.96448
16	Si	1	DZZ	0.00000	0.86503	0.04154	2.96448
17	Si	1	DXY	-0.18643	0.00000	0.00000	0.00000
18	Si	1	DXZ	0.98247	0.00000	0.00000	0.00000
19	Si	1	DYZ	0.00000	0.04797	-0.99885	0.00000

Beta Spin Molecular Orbital Coefficients

MO:				1	2	3	4	5
Eigenvalues:				-68.75612	-6.48926	-4.58487	-4.58487	-4.56819
				A	A	A	A	A
1	Si	1	S	0.98618	0.28630	0.00000	0.00000	0.00000
2	Si	1	S	0.06076	-0.97189	0.00000	0.00000	0.00000
3	Si	1	PX	0.00000	0.00000	0.00000	0.00000	0.97632
4	Si	1	PY	0.00000	0.00000	-0.93115	-0.29088	0.00000
5	Si	1	PZ	0.00000	0.00000	-0.29088	0.93115	0.00000
6	Si	1	S	-0.10273	-0.30734	0.00000	0.00000	0.00000
7	Si	1	PX	0.00000	0.00000	0.00000	0.00000	0.08296
8	Si	1	PY	0.00000	0.00000	-0.08156	-0.02548	0.00000
9	Si	1	PZ	0.00000	0.00000	-0.02548	0.08156	0.00000
10	Si	1	S	-0.00350	0.01837	0.00000	0.00000	0.00000
11	Si	1	PX	0.00000	0.00000	0.00000	0.00000	-0.02569
12	Si	1	PY	0.00000	0.00000	0.02512	0.00785	0.00000
13	Si	1	PZ	0.00000	0.00000	0.00785	-0.02512	0.00000
14	Si	1	DXX	0.04262	0.09810	0.00000	0.00000	0.00000
15	Si	1	DYY	0.04262	0.09665	0.00000	0.00000	0.00000
16	Si	1	DZZ	0.04262	0.09665	0.00000	0.00000	0.00000
17	Si	1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Si	1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Si	1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:				6	7	8	9	10
Eigenvalues:				-0.79421	-0.25135	-0.25135	-0.20222	0.16630
				A	A	A	A	A
1	Si	1	S	0.07088	0.00000	0.00000	0.00000	-0.05736
2	Si	1	S	-0.36221	0.00000	0.00000	0.00000	0.13759
3	Si	1	PX	0.00000	0.00000	0.00000	0.20116	0.00000
4	Si	1	PY	0.00000	0.05573	-0.20759	0.00000	0.00000
5	Si	1	PZ	0.00000	-0.20759	-0.05573	0.00000	0.00000
6	Si	1	S	0.51170	0.00000	0.00000	0.00000	-1.54761
7	Si	1	PX	0.00000	0.00000	0.00000	-0.38986	0.00000
8	Si	1	PY	0.00000	-0.11342	0.42254	0.00000	0.00000
9	Si	1	PZ	0.00000	0.42254	0.11342	0.00000	0.00000
10	Si	1	S	0.52822	0.00000	0.00000	0.00000	1.72644
11	Si	1	PX	0.00000	0.00000	0.00000	-0.71379	0.00000
12	Si	1	PY	0.00000	-0.17439	0.64964	0.00000	0.00000
13	Si	1	PZ	0.00000	0.64964	0.17439	0.00000	0.00000
14	Si	1	DXX	-0.02170	0.00000	0.00000	0.00000	-0.04666

15	Si	1 DYY	0.04315	0.00000	0.00000	0.00000	-0.10865
16	Si	1 DZZ	0.04315	0.00000	0.00000	0.00000	-0.10865
17	Si	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Si	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Si	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:			11	12	13	14	15
Eigenvalues:			0.24798	0.24798	0.28668	0.48896	0.48896
			A	A	A	A	A
1	Si	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2	Si	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3	Si	1 PX	0.00000	0.00000	-0.34497	0.00000	0.00000
4	Si	1 PY	-0.33026	-0.07574	0.00000	0.00000	0.00000
5	Si	1 PZ	-0.07574	0.33026	0.00000	0.00000	0.00000
6	Si	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7	Si	1 PX	0.00000	0.00000	1.32632	0.00000	0.00000
8	Si	1 PY	1.27804	0.29310	0.00000	0.00000	0.00000
9	Si	1 PZ	0.29310	-1.27804	0.00000	0.00000	0.00000
10	Si	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11	Si	1 PX	0.00000	0.00000	-1.12474	0.00000	0.00000
12	Si	1 PY	-1.12071	-0.25702	0.00000	0.00000	0.00000
13	Si	1 PZ	-0.25702	1.12071	0.00000	0.00000	0.00000
14	Si	1 DXX	0.00000	0.00000	0.00000	0.00000	0.00000
15	Si	1 DYY	0.00000	0.00000	0.00000	-0.86583	0.01859
16	Si	1 DZZ	0.00000	0.00000	0.00000	0.86583	-0.01859
17	Si	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Si	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Si	1 DYZ	0.00000	0.00000	0.00000	0.02146	0.99977

MO:			16	17	18	19
Eigenvalues:			0.53097	0.53097	0.54729	2.24464
			A	A	A	A
1	Si	1 S	0.00000	0.00000	-0.00580	0.13118
2	Si	1 S	0.00000	0.00000	0.02551	-1.04801
3	Si	1 PX	0.00000	0.00000	0.00000	0.00000
4	Si	1 PY	0.00000	0.00000	0.00000	0.00000
5	Si	1 PZ	0.00000	0.00000	0.00000	0.00000
6	Si	1 S	0.00000	0.00000	-0.11709	6.32901
7	Si	1 PX	0.00000	0.00000	0.00000	0.00000
8	Si	1 PY	0.00000	0.00000	0.00000	0.00000
9	Si	1 PZ	0.00000	0.00000	0.00000	0.00000
10	Si	1 S	0.00000	0.00000	0.04590	0.56091
11	Si	1 PX	0.00000	0.00000	0.00000	0.00000
12	Si	1 PY	0.00000	0.00000	0.00000	0.00000
13	Si	1 PZ	0.00000	0.00000	0.00000	0.00000
14	Si	1 DXX	0.00000	0.00000	-0.98836	-2.96876
15	Si	1 DYY	0.00000	0.00000	0.50893	-2.96153
16	Si	1 DZZ	0.00000	0.00000	0.50893	-2.96153
17	Si	1 DXY	0.95308	-0.30273	0.00000	0.00000
18	Si	1 DXZ	0.30273	0.95308	0.00000	0.00000
19	Si	1 DYZ	0.00000	0.00000	0.00000	0.00000

** Archive file written to unit 12 **

Total Cpu time: 0 mins. 1.27 secs.
Total Wall time: 0 mins. 2.08 secs.

```
  Calculation finished: Fri Sep 18 13:34:29 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:35:58 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  14
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  3

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    P  P1          -0.0000001    -0.0828409    -0.2012426

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.13E-06 in   6 cycles  <S**2> = 2.0076

  E(HF)  =    -338.6924885 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -79.91524   -7.90443   -5.79993   -5.79993   -5.78456

                        A         A         A         A         A
   1 P   1 S        -0.98557   -0.29193    0.00000    0.00000    0.00000
   2 P   1 S        -0.06550    0.95666    0.00000    0.00000    0.00000
   3 P   1 PX        0.00000    0.00000    0.32433    0.91963    0.00000
   4 P   1 PY        0.00000    0.00000   -0.91963    0.32433    0.00000
   5 P   1 PZ        0.00000    0.00000    0.00000    0.00000   -0.97352
   6 P   1 S         0.09021    0.29681    0.00000    0.00000    0.00000
   7 P   1 PX        0.00000    0.00000    0.02693    0.07636    0.00000
   8 P   1 PY        0.00000    0.00000   -0.07636    0.02693    0.00000
   9 P   1 PZ        0.00000    0.00000    0.00000    0.00000   -0.08599
  10 P   1 S         0.00746   -0.00821    0.00000    0.00000    0.00000
  11 P   1 PX        0.00000    0.00000   -0.00770   -0.02182    0.00000
  12 P   1 PY        0.00000    0.00000    0.02182   -0.00770    0.00000
  13 P   1 PZ        0.00000    0.00000    0.00000    0.00000    0.02510
  14 P   1 DXX      -0.03784   -0.09061    0.00000    0.00000    0.00000
  15 P   1 DYY      -0.03784   -0.09061    0.00000    0.00000    0.00000
  16 P   1 DZZ      -0.03787   -0.09093    0.00000    0.00000    0.00000
  17 P   1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 P   1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 P   1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:		6	7	8	9	10
Eigenvalues:		-1.13551	-0.72469	-0.72469	-0.34455	0.20650
		A	A	A	A	A
1 P	1 S	0.07598	0.00000	0.00000	0.00000	0.05867
2 P	1 S	-0.39859	0.00000	0.00000	0.00000	-0.17834
3 P	1 PX	0.00000	-0.25678	0.11599	0.00000	0.00000
4 P	1 PY	0.00000	-0.11599	-0.25678	0.00000	0.00000
5 P	1 PZ	0.00000	0.00000	0.00000	0.24298	0.00000
6 P	1 S	0.49740	0.00000	0.00000	0.00000	1.50264
7 P	1 PX	0.00000	0.58613	-0.26475	0.00000	0.00000
8 P	1 PY	0.00000	0.26475	0.58613	0.00000	0.00000
9 P	1 PZ	0.00000	0.00000	0.00000	-0.48788	0.00000
10 P	1 S	0.50750	0.00000	0.00000	0.00000	-1.78974
11 P	1 PX	0.00000	0.44105	-0.19922	0.00000	0.00000
12 P	1 PY	0.00000	0.19922	0.44105	0.00000	0.00000
13 P	1 PZ	0.00000	0.00000	0.00000	-0.63156	0.00000
14 P	1 DXX	0.06139	0.00000	0.00000	0.00000	0.14309
15 P	1 DYY	0.06139	0.00000	0.00000	0.00000	0.14309
16 P	1 DZZ	-0.00216	0.00000	0.00000	0.00000	0.13409
17 P	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18 P	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 P	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.29244	0.29244	0.32715	0.48354	0.48354
		A	A	A	A	A
1 P	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 P	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 P	1 PX	-0.30608	0.09141	0.00000	0.00000	0.00000
4 P	1 PY	-0.09141	-0.30608	0.00000	0.00000	0.00000
5 P	1 PZ	0.00000	0.00000	-0.35434	0.00000	0.00000
6 P	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 P	1 PX	1.17944	-0.35224	0.00000	0.00000	0.00000
8 P	1 PY	0.35224	1.17944	0.00000	0.00000	0.00000
9 P	1 PZ	0.00000	0.00000	1.29997	0.00000	0.00000
10 P	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 P	1 PX	-1.18646	0.35434	0.00000	0.00000	0.00000
12 P	1 PY	-0.35434	-1.18646	0.00000	0.00000	0.00000
13 P	1 PZ	0.00000	0.00000	-1.16983	0.00000	0.00000
14 P	1 DXX	0.00000	0.00000	0.00000	0.83462	-0.23109
15 P	1 DYY	0.00000	0.00000	0.00000	-0.83462	0.23109
16 P	1 DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
17 P	1 DXY	0.00000	0.00000	0.00000	-0.26684	-0.96374
18 P	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 P	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		16	17	18	19
Eigenvalues:		0.51201	0.51201	0.52362	2.62007
		A	A	A	A
1 P	1 S	0.00000	0.00000	0.00355	-0.12515
2 P	1 S	0.00000	0.00000	-0.01834	1.21951
3 P	1 PX	0.00000	0.00000	0.00000	0.00000
4 P	1 PY	0.00000	0.00000	0.00000	0.00000
5 P	1 PZ	0.00000	0.00000	0.00000	0.00000

6	P	1	S	0.00000	0.00000	0.03267	-5.36591
7	P	1	PX	0.00000	0.00000	0.00000	0.00000
8	P	1	PY	0.00000	0.00000	0.00000	0.00000
9	P	1	PZ	0.00000	0.00000	0.00000	0.00000
10	P	1	S	0.00000	0.00000	0.01118	-0.85823
11	P	1	PX	0.00000	0.00000	0.00000	0.00000
12	P	1	PY	0.00000	0.00000	0.00000	0.00000
13	P	1	PZ	0.00000	0.00000	0.00000	0.00000
14	P	1	DXX	0.00000	0.00000	-0.49823	2.62024
15	P	1	DYY	0.00000	0.00000	-0.49823	2.62024
16	P	1	DZZ	0.00000	0.00000	1.00039	2.62093
17	P	1	DXY	0.00000	0.00000	0.00000	0.00000
18	P	1	DXZ	-0.62315	0.78210	0.00000	0.00000
19	P	1	DYZ	-0.78210	-0.62315	0.00000	0.00000

Beta Spin Molecular Orbital Coefficients

MO:				1	2	3	4	5
Eigenvalues:				-79.89943	-7.88718	-5.77705	-5.75660	-5.75660
				A	A	A	A	A
1	P	1	S	0.98562	0.29192	0.00000	0.00000	0.00000
2	P	1	S	0.06526	-0.95677	0.00000	0.00000	0.00000
3	P	1	PX	0.00000	0.00000	0.00000	-0.92694	0.30052
4	P	1	PY	0.00000	0.00000	0.00000	-0.30052	-0.92694
5	P	1	PZ	0.00000	0.00000	0.97368	0.00000	0.00000
6	P	1	S	-0.08974	-0.29886	0.00000	0.00000	0.00000
7	P	1	PX	0.00000	0.00000	0.00000	-0.07928	0.02570
8	P	1	PY	0.00000	0.00000	0.00000	-0.02570	-0.07928
9	P	1	PZ	0.00000	0.00000	0.08560	0.00000	0.00000
10	P	1	S	-0.00743	0.00828	0.00000	0.00000	0.00000
11	P	1	PX	0.00000	0.00000	0.00000	0.02348	-0.00761
12	P	1	PY	0.00000	0.00000	0.00000	0.00761	0.02348
13	P	1	PZ	0.00000	0.00000	-0.02525	0.00000	0.00000
14	P	1	DXX	0.03767	0.09303	0.00000	0.00000	0.00000
15	P	1	DYY	0.03767	0.09303	0.00000	0.00000	0.00000
16	P	1	DZZ	0.03767	0.09160	0.00000	0.00000	0.00000
17	P	1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	P	1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	P	1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:				6	7	8	9	10
Eigenvalues:				-0.93366	-0.30995	-0.25305	-0.25305	0.24872
				A	A	A	A	A
1	P	1	S	0.07523	0.00000	0.00000	0.00000	0.05879
2	P	1	S	-0.40202	0.00000	0.00000	0.00000	-0.17630
3	P	1	PX	0.00000	0.00000	-0.18381	0.12987	0.00000
4	P	1	PY	0.00000	0.00000	-0.12987	-0.18381	0.00000
5	P	1	PZ	0.00000	0.23749	0.00000	0.00000	0.00000
6	P	1	S	0.51131	0.00000	0.00000	0.00000	1.47722
7	P	1	PX	0.00000	0.00000	0.35040	-0.24757	0.00000
8	P	1	PY	0.00000	0.00000	0.24757	0.35040	0.00000
9	P	1	PZ	0.00000	-0.46945	0.00000	0.00000	0.00000
10	P	1	S	0.54014	0.00000	0.00000	0.00000	-1.78543
11	P	1	PX	0.00000	0.00000	0.55824	-0.39442	0.00000
12	P	1	PY	0.00000	0.00000	0.39442	0.55824	0.00000
13	P	1	PZ	0.00000	-0.64806	0.00000	0.00000	0.00000
14	P	1	DXX	-0.00123	0.00000	0.00000	0.00000	0.12986

```
15 P   1 DYY      -0.00123    0.00000    0.00000    0.00000    0.12986
16 P   1 DZZ       0.06336    0.00000    0.00000    0.00000    0.20550
17 P   1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
18 P   1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
19 P   1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000

MO:                  11         12         13         14         15

Eigenvalues:       0.34171    0.38436    0.38436    0.58617    0.59924

                      A          A          A          A          A
 1 P   1 S         0.00000    0.00000    0.00000   -0.00649    0.00000
 2 P   1 S         0.00000    0.00000    0.00000    0.03067    0.00000
 3 P   1 PX        0.00000   -0.30598   -0.19628    0.00000    0.00000
 4 P   1 PY        0.00000   -0.19628    0.30598    0.00000    0.00000
 5 P   1 PZ       -0.35762    0.00000    0.00000    0.00000    0.00000
 6 P   1 S         0.00000    0.00000    0.00000   -0.12049    0.00000
 7 P   1 PX        0.00000    1.11167    0.71310    0.00000    0.00000
 8 P   1 PY        0.00000    0.71310   -1.11167    0.00000    0.00000
 9 P   1 PZ        1.30677    0.00000    0.00000    0.00000    0.00000
10 P   1 S         0.00000    0.00000    0.00000    0.06324    0.00000
11 P   1 PX        0.00000   -0.95977   -0.61566    0.00000    0.00000
12 P   1 PY        0.00000   -0.61566    0.95977    0.00000    0.00000
13 P   1 PZ       -1.16077    0.00000    0.00000    0.00000    0.00000
14 P   1 DXX       0.00000    0.00000    0.00000   -0.49606    0.00000
15 P   1 DYY       0.00000    0.00000    0.00000   -0.49606    0.00000
16 P   1 DZZ       0.00000    0.00000    0.00000    1.00062    0.00000
17 P   1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
18 P   1 DXZ       0.00000    0.00000    0.00000    0.00000    0.19797
19 P   1 DYZ       0.00000    0.00000    0.00000    0.00000    0.98021

MO:                  16         17         18         19

Eigenvalues:       0.59924    0.64670    0.64670    2.65623

                      A          A          A          A
 1 P   1 S         0.00000    0.00000    0.00000   -0.12508
 2 P   1 S         0.00000    0.00000    0.00000    1.21836
 3 P   1 PX        0.00000    0.00000    0.00000    0.00000
 4 P   1 PY        0.00000    0.00000    0.00000    0.00000
 5 P   1 PZ        0.00000    0.00000    0.00000    0.00000
 6 P   1 S         0.00000    0.00000    0.00000   -5.37030
 7 P   1 PX        0.00000    0.00000    0.00000    0.00000
 8 P   1 PY        0.00000    0.00000    0.00000    0.00000
 9 P   1 PZ        0.00000    0.00000    0.00000    0.00000
10 P   1 S         0.00000    0.00000    0.00000   -0.84495
11 P   1 PX        0.00000    0.00000    0.00000    0.00000
12 P   1 PY        0.00000    0.00000    0.00000    0.00000
13 P   1 PZ        0.00000    0.00000    0.00000    0.00000
14 P   1 DXX       0.00000   -0.83808    0.21823    2.62197
15 P   1 DYY       0.00000    0.83808   -0.21823    2.62197
16 P   1 DZZ       0.00000    0.00000    0.00000    2.61543
17 P   1 DXY       0.00000    0.25199    0.96773    0.00000
18 P   1 DXZ       0.98021    0.00000    0.00000    0.00000
19 P   1 DYZ      -0.19797    0.00000    0.00000    0.00000

  ** Archive file written to unit 12 **

Total Cpu time:        0 mins.  1.29 secs.
Total Wall time:       0 mins.  1.77 secs.
```

```
  Calculation finished: Fri Sep 18 13:36:00 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:37:09 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  15
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  4

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    S  S1          -0.0000001     1.7810652    -2.3970894

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.57E-05 in   5 cycles  <S**2> = 3.7509

  E(HF)  =    -395.2924871 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:     -91.90745   -9.41623   -7.10243   -7.10243   -7.10243

                        A         A         A         A         A
   1 S   1 S         0.98492    0.29744    0.00000    0.00000    0.00000
   2 S   1 S         0.07349   -0.93727    0.00000    0.00000    0.00000
   3 S   1 PX        0.00000    0.00000    0.53238    0.36086   -0.73287
   4 S   1 PY        0.00000    0.00000    0.73994    0.15764    0.61514
   5 S   1 PZ        0.00000    0.00000    0.34614   -0.89201   -0.18777
   6 S   1 S        -0.09594   -0.30639    0.00000    0.00000    0.00000
   7 S   1 PX        0.00000    0.00000    0.04279    0.02900   -0.05890
   8 S   1 PY        0.00000    0.00000    0.05947    0.01267    0.04944
   9 S   1 PZ        0.00000    0.00000    0.02782   -0.07169   -0.01509
  10 S   1 S        -0.00584    0.01328    0.00000    0.00000    0.00000
  11 S   1 PX        0.00000    0.00000   -0.01205   -0.00817    0.01658
  12 S   1 PY        0.00000    0.00000   -0.01674   -0.00357   -0.01392
  13 S   1 PZ        0.00000    0.00000   -0.00783    0.02019    0.00425
  14 S   1 DXX       0.03856    0.08837    0.00000    0.00000    0.00000
  15 S   1 DYY       0.03856    0.08837    0.00000    0.00000    0.00000
  16 S   1 DZZ       0.03856    0.08837    0.00000    0.00000    0.00000
  17 S   1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 S   1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 S   1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:		6	7	8	9	10
Eigenvalues:		-1.41066	-0.86266	-0.86266	-0.86266	0.20397
		A	A	A	A	A
1 S	1 S	0.08051	0.00000	0.00000	0.00000	-0.05742
2 S	1 S	-0.44954	0.00000	0.00000	0.00000	0.26676
3 S	1 PX	0.00000	-0.19963	-0.01184	-0.22670	0.00000
4 S	1 PY	0.00000	-0.20481	0.13960	0.17306	0.00000
5 S	1 PZ	0.00000	-0.09791	-0.26787	0.10021	0.00000
6 S	1 S	0.59831	0.00000	0.00000	0.00000	-1.50842
7 S	1 PX	0.00000	0.46494	0.02758	0.52799	0.00000
8 S	1 PY	0.00000	0.47701	-0.32513	-0.40306	0.00000
9 S	1 PZ	0.00000	0.22803	0.62389	-0.23340	0.00000
10 S	1 S	0.42868	0.00000	0.00000	0.00000	1.79504
11 S	1 PX	0.00000	0.28338	0.01681	0.32181	0.00000
12 S	1 PY	0.00000	0.29073	-0.19817	-0.24567	0.00000
13 S	1 PZ	0.00000	0.13898	0.38026	-0.14225	0.00000
14 S	1 DXX	0.03779	0.00000	0.00000	0.00000	-0.13482
15 S	1 DYY	0.03779	0.00000	0.00000	0.00000	-0.13482
16 S	1 DZZ	0.03779	0.00000	0.00000	0.00000	-0.13482
17 S	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18 S	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 S	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.31898	0.31898	0.31898	0.53060	0.53060
		A	A	A	A	A
1 S	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 S	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 S	1 PX	0.23093	-0.04752	-0.21062	0.00000	0.00000
4 S	1 PY	0.20949	-0.02537	0.23541	0.00000	0.00000
5 S	1 PZ	-0.05229	-0.31152	0.01296	0.00000	0.00000
6 S	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 S	1 PX	-0.85829	0.17662	0.78282	0.00000	0.00000
8 S	1 PY	-0.77861	0.09429	-0.87495	0.00000	0.00000
9 S	1 PZ	0.19434	1.15783	-0.04816	0.00000	0.00000
10 S	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 S	1 PX	0.90113	-0.18544	-0.82189	0.00000	0.00000
12 S	1 PY	0.81747	-0.09900	0.91862	0.00000	0.00000
13 S	1 PZ	-0.20404	-1.21562	0.05057	0.00000	0.00000
14 S	1 DXX	0.00000	0.00000	0.00000	-0.26045	0.94217
15 S	1 DYY	0.00000	0.00000	0.00000	0.95673	-0.22880
16 S	1 DZZ	0.00000	0.00000	0.00000	-0.69628	-0.71338
17 S	1 DXY	0.00000	0.00000	0.00000	-0.06505	0.04270
18 S	1 DXZ	0.00000	0.00000	0.00000	-0.07690	0.17134
19 S	1 DYZ	0.00000	0.00000	0.00000	-0.10587	0.05345

MO:		16	17	18	19
Eigenvalues:		0.53060	0.53060	0.53060	3.27013
		A	A	A	A
1 S	1 S	0.00000	0.00000	0.00000	-0.12186
2 S	1 S	0.00000	0.00000	0.00000	1.50558
3 S	1 PX	0.00000	0.00000	0.00000	0.00000
4 S	1 PY	0.00000	0.00000	0.00000	0.00000
5 S	1 PZ	0.00000	0.00000	0.00000	0.00000

6	S	1	S	0.00000	0.00000	0.00000	-5.28048
7	S	1	PX	0.00000	0.00000	0.00000	0.00000
8	S	1	PY	0.00000	0.00000	0.00000	0.00000
9	S	1	PZ	0.00000	0.00000	0.00000	0.00000
10	S	1	S	0.00000	0.00000	0.00000	-0.75668
11	S	1	PX	0.00000	0.00000	0.00000	0.00000
12	S	1	PY	0.00000	0.00000	0.00000	0.00000
13	S	1	PZ	0.00000	0.00000	0.00000	0.00000
14	S	1	DXX	-0.11388	0.15041	0.09423	2.49412
15	S	1	DYY	0.14579	-0.08622	-0.06026	2.49412
16	S	1	DZZ	-0.03190	-0.06419	-0.03398	2.49412
17	S	1	DXY	0.42617	0.43657	-0.78849	0.00000
18	S	1	DXZ	0.07538	-0.87955	-0.43063	0.00000
19	S	1	DYZ	0.88837	-0.11406	0.42863	0.00000

Beta Spin Molecular Orbital Coefficients

MO:				1	2	3	4	5
Eigenvalues:				-91.87683	-9.38470	-7.04507	-7.04507	-7.04507
				A	A	A	A	A
1	S	1	S	-0.98500	-0.29745	0.00000	0.00000	0.00000
2	S	1	S	-0.07305	0.93748	0.00000	0.00000	0.00000
3	S	1	PX	0.00000	0.00000	0.47687	-0.40652	0.74617
4	S	1	PY	0.00000	0.00000	0.73135	-0.23925	-0.59775
5	S	1	PZ	0.00000	0.00000	0.43260	0.85260	0.18803
6	S	1	S	0.09514	0.30879	0.00000	0.00000	0.00000
7	S	1	PX	0.00000	0.00000	0.03944	-0.03362	0.06172
8	S	1	PY	0.00000	0.00000	0.06049	-0.01979	-0.04944
9	S	1	PZ	0.00000	0.00000	0.03578	0.07052	0.01555
10	S	1	S	0.00580	-0.01333	0.00000	0.00000	0.00000
11	S	1	PX	0.00000	0.00000	-0.01155	0.00984	-0.01807
12	S	1	PY	0.00000	0.00000	-0.01771	0.00579	0.01448
13	S	1	PZ	0.00000	0.00000	-0.01048	-0.02065	-0.00455
14	S	1	DXX	-0.03828	-0.09094	0.00000	0.00000	0.00000
15	S	1	DYY	-0.03828	-0.09094	0.00000	0.00000	0.00000
16	S	1	DZZ	-0.03828	-0.09094	0.00000	0.00000	0.00000
17	S	1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	S	1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	S	1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:				6	7	8	9	10
Eigenvalues:				-1.06850	-0.30948	-0.30948	-0.30948	0.27176
				A	A	A	A	A
1	S	1	S	-0.07858	0.00000	0.00000	0.00000	-0.05847
2	S	1	S	0.44946	0.00000	0.00000	0.00000	0.26680
3	S	1	PX	0.00000	0.09070	-0.22686	-0.00585	0.00000
4	S	1	PY	0.00000	-0.12691	-0.04548	-0.20384	0.00000
5	S	1	PZ	0.00000	-0.18813	-0.07869	0.13468	0.00000
6	S	1	S	-0.59459	0.00000	0.00000	0.00000	-1.48242
7	S	1	PX	0.00000	-0.18310	0.45799	0.01181	0.00000
8	S	1	PY	0.00000	0.25620	0.09182	0.41152	0.00000
9	S	1	PZ	0.00000	0.37981	0.15885	-0.27190	0.00000
10	S	1	S	-0.48455	0.00000	0.00000	0.00000	1.78823
11	S	1	PX	0.00000	-0.23499	0.58778	0.01515	0.00000
12	S	1	PY	0.00000	0.32881	0.11784	0.52814	0.00000
13	S	1	PZ	0.00000	0.48744	0.20387	-0.34896	0.00000
14	S	1	DXX	-0.01570	0.00000	0.00000	0.00000	-0.15582

15 S	1 DYY	-0.01570	0.00000	0.00000	0.00000	-0.15582
16 S	1 DZZ	-0.01570	0.00000	0.00000	0.00000	-0.15582
17 S	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18 S	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 S	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.42675	0.42675	0.42675	0.72237	0.72237
		A	A	A	A	A
1 S	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 S	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 S	1 PX	0.11599	0.26835	0.21787	0.00000	0.00000
4 S	1 PY	0.18090	0.14870	-0.27946	0.00000	0.00000
5 S	1 PZ	0.29454	-0.19700	0.08584	0.00000	0.00000
6 S	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 S	1 PX	-0.40648	-0.94042	-0.76353	0.00000	0.00000
8 S	1 PY	-0.63396	-0.52112	0.97935	0.00000	0.00000
9 S	1 PZ	-1.03221	0.69040	-0.30081	0.00000	0.00000
10 S	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 S	1 PX	0.36343	0.84081	0.68266	0.00000	0.00000
12 S	1 PY	0.56681	0.46592	-0.87561	0.00000	0.00000
13 S	1 PZ	0.92288	-0.61727	0.26895	0.00000	0.00000
14 S	1 DXX	0.00000	0.00000	0.00000	0.90568	-0.27403
15 S	1 DYY	0.00000	0.00000	0.00000	-0.70963	-0.60327
16 S	1 DZZ	0.00000	0.00000	0.00000	-0.19606	0.87731
17 S	1 DXY	0.00000	0.00000	0.00000	0.29479	-0.11152
18 S	1 DXZ	0.00000	0.00000	0.00000	0.06049	0.42238
19 S	1 DYZ	0.00000	0.00000	0.00000	0.03539	0.05798

MO:		16	17	18	19
Eigenvalues:		0.72237	0.72237	0.72237	3.33448
		A	A	A	A
1 S	1 S	0.00000	0.00000	0.00000	-0.12193
2 S	1 S	0.00000	0.00000	0.00000	1.50548
3 S	1 PX	0.00000	0.00000	0.00000	0.00000
4 S	1 PY	0.00000	0.00000	0.00000	0.00000
5 S	1 PZ	0.00000	0.00000	0.00000	0.00000
6 S	1 S	0.00000	0.00000	0.00000	-5.28813
7 S	1 PX	0.00000	0.00000	0.00000	0.00000
8 S	1 PY	0.00000	0.00000	0.00000	0.00000
9 S	1 PZ	0.00000	0.00000	0.00000	0.00000
10 S	1 S	0.00000	0.00000	0.00000	-0.73888
11 S	1 PX	0.00000	0.00000	0.00000	0.00000
12 S	1 PY	0.00000	0.00000	0.00000	0.00000
13 S	1 PZ	0.00000	0.00000	0.00000	0.00000
14 S	1 DXX	-0.20500	-0.04089	0.24686	2.49304
15 S	1 DYY	-0.22960	0.09203	-0.26703	2.49304
16 S	1 DZZ	0.43460	-0.05114	0.02017	2.49304
17 S	1 DXY	0.42511	0.24955	-0.81096	0.00000
18 S	1 DXZ	-0.77071	0.33094	-0.33827	0.00000
19 S	1 DYZ	-0.19029	-0.90537	-0.37346	0.00000

** Archive file written to unit 12 **

Total Cpu time: 0 mins. 1.12 secs.
Total Wall time: 0 mins. 1.82 secs.

```
  Calculation finished: Fri Sep 18 13:37:11 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:38:25 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  16
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  3

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Cl Cl1          0.0000000     2.8994087    -2.1997787

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.29E-05 in   5 cycles  <S**2> = 2.0061

  E(HF)  =    -456.9359368 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:    -104.76101  -11.05701   -8.53714   -8.53714   -8.50844

                        A         A         A         A         A
   1 Cl  1 S        -0.98444   -0.30211    0.00000    0.00000    0.00000
   2 Cl  1 S        -0.07577    0.92893    0.00000    0.00000    0.00000
   3 Cl  1 PX        0.00000    0.00000    0.00000    0.00000    0.97563
   4 Cl  1 PY        0.00000    0.00000    0.97483    0.02248    0.00000
   5 Cl  1 PZ        0.00000    0.00000   -0.02248    0.97483    0.00000
   6 Cl  1 S         0.08964    0.30335    0.00000    0.00000    0.00000
   7 Cl  1 PX        0.00000    0.00000    0.00000    0.00000    0.07490
   8 Cl  1 PY        0.00000    0.00000    0.07642    0.00176    0.00000
   9 Cl  1 PZ        0.00000    0.00000   -0.00176    0.07642    0.00000
  10 Cl  1 S         0.00599   -0.01252    0.00000    0.00000    0.00000
  11 Cl  1 PX        0.00000    0.00000    0.00000    0.00000   -0.02115
  12 Cl  1 PY        0.00000    0.00000   -0.02154   -0.00050    0.00000
  13 Cl  1 PZ        0.00000    0.00000    0.00050   -0.02154    0.00000
  14 Cl  1 DXX      -0.03544   -0.08581    0.00000    0.00000    0.00000
  15 Cl  1 DYY      -0.03544   -0.08447    0.00000    0.00000    0.00000
  16 Cl  1 DZZ      -0.03544   -0.08447    0.00000    0.00000    0.00000
  17 Cl  1 DXY       0.00000    0.00000    0.00000    0.00000    0.00000
  18 Cl  1 DXZ       0.00000    0.00000    0.00000    0.00000    0.00000
  19 Cl  1 DYZ       0.00000    0.00000    0.00000    0.00000    0.00000
```

MO:	6	7	8	9	10
Eigenvalues:	-1.59865	-0.99500	-0.99500	-0.91596	0.24539
	A	A	A	A	A
1 Cl 1 S	-0.08384	0.00000	0.00000	0.00000	-0.05654
2 Cl 1 S	0.48165	0.00000	0.00000	0.00000	0.28888
3 Cl 1 PX	0.00000	0.00000	0.00000	0.30916	0.00000
4 Cl 1 PY	0.00000	0.23306	-0.21477	0.00000	0.00000
5 Cl 1 PZ	0.00000	0.21477	0.23306	0.00000	0.00000
6 Cl 1 S	-0.65317	0.00000	0.00000	0.00000	-1.46171
7 Cl 1 PX	0.00000	0.00000	0.00000	-0.71760	0.00000
8 Cl 1 PY	0.00000	-0.54560	0.50277	0.00000	0.00000
9 Cl 1 PZ	0.00000	-0.50277	-0.54560	0.00000	0.00000
10 Cl 1 S	-0.39081	0.00000	0.00000	0.00000	1.82124
11 Cl 1 PX	0.00000	0.00000	0.00000	-0.41905	0.00000
12 Cl 1 PY	0.00000	-0.28901	0.26632	0.00000	0.00000
13 Cl 1 PZ	0.00000	-0.26632	-0.28901	0.00000	0.00000
14 Cl 1 DXX	-0.00088	0.00000	0.00000	0.00000	-0.12279
15 Cl 1 DYY	-0.05104	0.00000	0.00000	0.00000	-0.18312
16 Cl 1 DZZ	-0.05104	0.00000	0.00000	0.00000	-0.18312
17 Cl 1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18 Cl 1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 Cl 1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	11	12	13	14	15
Eigenvalues:	0.36706	0.36706	0.41136	0.57599	0.57599
	A	A	A	A	A
1 Cl 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 Cl 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 Cl 1 PX	0.00000	0.00000	-0.32109	0.00000	0.00000
4 Cl 1 PY	-0.30332	-0.08545	0.00000	0.00000	0.00000
5 Cl 1 PZ	0.08545	-0.30332	0.00000	0.00000	0.00000
6 Cl 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 Cl 1 PX	0.00000	0.00000	1.16191	0.00000	0.00000
8 Cl 1 PY	1.10348	0.31087	0.00000	0.00000	0.00000
9 Cl 1 PZ	-0.31087	1.10348	0.00000	0.00000	0.00000
10 Cl 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 Cl 1 PX	0.00000	0.00000	-1.22871	0.00000	0.00000
12 Cl 1 PY	-1.19092	-0.33551	0.00000	0.00000	0.00000
13 Cl 1 PZ	0.33551	-1.19092	0.00000	0.00000	0.00000
14 Cl 1 DXX	0.00000	0.00000	0.00000	0.00000	0.00000
15 Cl 1 DYY	0.00000	0.00000	0.00000	-0.86544	0.03179
16 Cl 1 DZZ	0.00000	0.00000	0.00000	0.86544	-0.03179
17 Cl 1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18 Cl 1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 Cl 1 DYZ	0.00000	0.00000	0.00000	0.03671	0.99933

MO:	16	17	18	19
Eigenvalues:	0.63381	0.63381	0.65562	3.77857
	A	A	A	A
1 Cl 1 S	0.00000	0.00000	-0.00524	0.12037
2 Cl 1 S	0.00000	0.00000	0.03244	-1.55453
3 Cl 1 PX	0.00000	0.00000	0.00000	0.00000
4 Cl 1 PY	0.00000	0.00000	0.00000	0.00000
5 Cl 1 PZ	0.00000	0.00000	0.00000	0.00000

6	Cl	1	S	0.00000	0.00000	-0.09818	4.84203
7	Cl	1	PX	0.00000	0.00000	0.00000	0.00000
8	Cl	1	PY	0.00000	0.00000	0.00000	0.00000
9	Cl	1	PZ	0.00000	0.00000	0.00000	0.00000
10	Cl	1	S	0.00000	0.00000	0.05750	0.78459
11	Cl	1	PX	0.00000	0.00000	0.00000	0.00000
12	Cl	1	PY	0.00000	0.00000	0.00000	0.00000
13	Cl	1	PZ	0.00000	0.00000	0.00000	0.00000
14	Cl	1	DXX	0.00000	0.00000	-0.99811	-2.30262
15	Cl	1	DYY	0.00000	0.00000	0.49982	-2.29731
16	Cl	1	DZZ	0.00000	0.00000	0.49982	-2.29731
17	Cl	1	DXY	0.70932	0.70489	0.00000	0.00000
18	Cl	1	DXZ	-0.70489	0.70932	0.00000	0.00000
19	Cl	1	DYZ	0.00000	0.00000	0.00000	0.00000

Beta Spin Molecular Orbital Coefficients

MO:				1	2	3	4	5
Eigenvalues:				-104.73583	-11.03223	-8.49545	-8.47590	-8.47590
				A	A	A	A	A
1	Cl	1	S	0.98450	0.30214	0.00000	0.00000	0.00000
2	Cl	1	S	0.07545	-0.92930	0.00000	0.00000	0.00000
3	Cl	1	PX	0.00000	0.00000	-0.97578	0.00000	0.00000
4	Cl	1	PY	0.00000	0.00000	0.00000	0.97400	-0.02413
5	Cl	1	PZ	0.00000	0.00000	0.00000	-0.02413	-0.97400
6	Cl	1	S	-0.08911	-0.30409	0.00000	0.00000	0.00000
7	Cl	1	PX	0.00000	0.00000	-0.07451	0.00000	0.00000
8	Cl	1	PY	0.00000	0.00000	0.00000	0.07886	-0.00195
9	Cl	1	PZ	0.00000	0.00000	0.00000	-0.00195	-0.07886
10	Cl	1	S	-0.00597	0.01245	0.00000	0.00000	0.00000
11	Cl	1	PX	0.00000	0.00000	0.02125	0.00000	0.00000
12	Cl	1	PY	0.00000	0.00000	0.00000	-0.02295	0.00057
13	Cl	1	PZ	0.00000	0.00000	0.00000	0.00057	0.02295
14	Cl	1	DXX	0.03524	0.08605	0.00000	0.00000	0.00000
15	Cl	1	DYY	0.03527	0.08653	0.00000	0.00000	0.00000
16	Cl	1	DZZ	0.03527	0.08653	0.00000	0.00000	0.00000
17	Cl	1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18	Cl	1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19	Cl	1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:				6	7	8	9	10
Eigenvalues:				-1.34397	-0.86433	-0.39855	-0.39855	0.29293
				A	A	A	A	A
1	Cl	1	S	0.08221	0.00000	0.00000	0.00000	-0.05756
2	Cl	1	S	-0.47859	0.00000	0.00000	0.00000	0.29040
3	Cl	1	PX	0.00000	0.30363	0.00000	0.00000	0.00000
4	Cl	1	PY	0.00000	0.00000	-0.26479	0.01729	0.00000
5	Cl	1	PZ	0.00000	0.00000	0.01729	0.26479	0.00000
6	Cl	1	S	0.64013	0.00000	0.00000	0.00000	-1.44953
7	Cl	1	PX	0.00000	-0.69916	0.00000	0.00000	0.00000
8	Cl	1	PY	0.00000	0.00000	0.55521	-0.03625	0.00000
9	Cl	1	PZ	0.00000	0.00000	-0.03625	-0.55521	0.00000
10	Cl	1	S	0.43115	0.00000	0.00000	0.00000	1.81816
11	Cl	1	PX	0.00000	-0.43843	0.00000	0.00000	0.00000
12	Cl	1	PY	0.00000	0.00000	0.57771	-0.03772	0.00000
13	Cl	1	PZ	0.00000	0.00000	-0.03772	-0.57771	0.00000
14	Cl	1	DXX	0.06301	0.00000	0.00000	0.00000	-0.18432

15 Cl	1 DYY	0.00252	0.00000	0.00000	0.00000	-0.17307
16 Cl	1 DZZ	0.00252	0.00000	0.00000	0.00000	-0.17307
17 Cl	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
18 Cl	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
19 Cl	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.42949	0.47236	0.47236	0.73706	0.74619
		A	A	A	A	A
1 Cl	1 S	0.00000	0.00000	0.00000	-0.00359	0.00000
2 Cl	1 S	0.00000	0.00000	0.00000	0.02064	0.00000
3 Cl	1 PX	0.32588	0.00000	0.00000	0.00000	0.00000
4 Cl	1 PY	0.00000	0.35652	-0.06132	0.00000	0.00000
5 Cl	1 PZ	0.00000	-0.06132	-0.35652	0.00000	0.00000
6 Cl	1 S	0.00000	0.00000	0.00000	-0.03506	0.00000
7 Cl	1 PX	-1.17313	0.00000	0.00000	0.00000	0.00000
8 Cl	1 PY	0.00000	-1.22887	0.21136	0.00000	0.00000
9 Cl	1 PZ	0.00000	0.21136	1.22887	0.00000	0.00000
10 Cl	1 S	0.00000	0.00000	0.00000	-0.00347	0.00000
11 Cl	1 PX	1.22193	0.00000	0.00000	0.00000	0.00000
12 Cl	1 PY	0.00000	1.14511	-0.19695	0.00000	0.00000
13 Cl	1 PZ	0.00000	-0.19695	-1.14511	0.00000	0.00000
14 Cl	1 DXX	0.00000	0.00000	0.00000	0.99611	0.00000
15 Cl	1 DYY	0.00000	0.00000	0.00000	-0.50263	0.00000
16 Cl	1 DZZ	0.00000	0.00000	0.00000	-0.50263	0.00000
17 Cl	1 DXY	0.00000	0.00000	0.00000	0.00000	-0.06449
18 Cl	1 DXZ	0.00000	0.00000	0.00000	0.00000	-0.99792
19 Cl	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		16	17	18	19
Eigenvalues:		0.74619	0.78100	0.78100	3.82847
		A	A	A	A
1 Cl	1 S	0.00000	0.00000	0.00000	0.12051
2 Cl	1 S	0.00000	0.00000	0.00000	-1.55519
3 Cl	1 PX	0.00000	0.00000	0.00000	0.00000
4 Cl	1 PY	0.00000	0.00000	0.00000	0.00000
5 Cl	1 PZ	0.00000	0.00000	0.00000	0.00000
6 Cl	1 S	0.00000	0.00000	0.00000	4.84826
7 Cl	1 PX	0.00000	0.00000	0.00000	0.00000
8 Cl	1 PY	0.00000	0.00000	0.00000	0.00000
9 Cl	1 PZ	0.00000	0.00000	0.00000	0.00000
10 Cl	1 S	0.00000	0.00000	0.00000	0.77261
11 Cl	1 PX	0.00000	0.00000	0.00000	0.00000
12 Cl	1 PY	0.00000	0.00000	0.00000	0.00000
13 Cl	1 PZ	0.00000	0.00000	0.00000	0.00000
14 Cl	1 DXX	0.00000	0.00000	0.00000	-2.29852
15 Cl	1 DYY	0.00000	-0.86603	-0.00041	-2.29797
16 Cl	1 DZZ	0.00000	0.86603	0.00041	-2.29797
17 Cl	1 DXY	-0.99792	0.00000	0.00000	0.00000
18 Cl	1 DXZ	0.06449	0.00000	0.00000	0.00000
19 Cl	1 DYZ	0.00000	-0.00047	1.00000	0.00000

** Archive file written to unit 12 **

Total Cpu time: 0 mins. 1.14 secs.
Total Wall time: 0 mins. 1.67 secs.

```
  Calculation finished: Fri Sep 18 13:38:26 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:40:06 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   5
     1 S shells
     3 SP shells
     1 6D shells
  Number of basis functions:  19
  Number of electrons:  17
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Ar Ar1         -0.0000002    -0.3934908    -1.9923078

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.25E-11 in  11 cycles  <S**2> = 0.7551

  E(HF)  =    -523.9070140 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:    -118.45295  -12.80927  -10.08177  -10.04918  -10.04918

                        A         A         A         A         A
   1 Ar  1 S         0.98405    0.30618    0.00000    0.00000    0.00000
   2 Ar  1 S         0.07610   -0.92421    0.00000    0.00000    0.00000
   3 Ar  1 PX        0.00000    0.00000    0.66128    0.10228    0.70944
   4 Ar  1 PY        0.00000    0.00000   -0.20551    0.95198    0.05451
   5 Ar  1 PZ        0.00000    0.00000    0.68629    0.18652   -0.66726
   6 Ar  1 S        -0.08069   -0.29645    0.00000    0.00000    0.00000
   7 Ar  1 PX        0.00000    0.00000    0.05109    0.00775    0.05374
   8 Ar  1 PY        0.00000    0.00000   -0.01588    0.07211    0.00413
   9 Ar  1 PZ        0.00000    0.00000    0.05302    0.01413   -0.05055
  10 Ar  1 S        -0.00717    0.00810    0.00000    0.00000    0.00000
  11 Ar  1 PX        0.00000    0.00000   -0.01441   -0.00219   -0.01519
  12 Ar  1 PY        0.00000    0.00000    0.00448   -0.02038   -0.00117
  13 Ar  1 PZ        0.00000    0.00000   -0.01496   -0.00399    0.01428
  14 Ar  1 DXX       0.03188    0.08170    0.00000    0.00000    0.00000
  15 Ar  1 DYY       0.03188    0.08223    0.00000    0.00000    0.00000
  16 Ar  1 DZZ       0.03188    0.08166    0.00000    0.00000    0.00000
  17 Ar  1 DXY       0.00000    0.00021    0.00000    0.00000    0.00000
  18 Ar  1 DXZ       0.00000   -0.00070    0.00000    0.00000    0.00000
  19 Ar  1 DYZ       0.00000    0.00022    0.00000    0.00000    0.00000
```

MO:	6	7	8	9	10
Eigenvalues:	-1.78267	-1.12942	-1.04334	-1.04334	0.30579
	A	A	A	A	A
1 Ar 1 S	0.08645	0.00000	0.00000	0.00000	0.05611
2 Ar 1 S	-0.50361	0.00000	0.00000	0.00000	-0.29478
3 Ar 1 PX	0.00000	-0.22237	-0.22817	0.05870	0.00000
4 Ar 1 PY	0.00000	0.06911	0.01610	0.31301	0.00000
5 Ar 1 PZ	0.00000	-0.23078	0.22468	0.03717	0.00000
6 Ar 1 S	0.67940	0.00000	0.00000	0.00000	1.42593
7 Ar 1 PX	0.00000	0.51815	0.52781	-0.13578	0.00000
8 Ar 1 PY	0.00000	-0.16103	-0.03725	-0.72406	0.00000
9 Ar 1 PZ	0.00000	0.53774	-0.51973	-0.08599	0.00000
10 Ar 1 S	0.37505	0.00000	0.00000	0.00000	-1.85793
11 Ar 1 PX	0.00000	0.25227	0.28189	-0.07251	0.00000
12 Ar 1 PY	0.00000	-0.07840	-0.01989	-0.38670	0.00000
13 Ar 1 PZ	0.00000	0.26181	-0.27758	-0.04593	0.00000
14 Ar 1 DXX	0.03904	0.00000	0.00000	0.00000	0.20336
15 Ar 1 DYY	0.01842	0.00000	0.00000	0.00000	0.17478
16 Ar 1 DZZ	0.04079	0.00000	0.00000	0.00000	0.20580
17 Ar 1 DXY	-0.00819	0.00000	0.00000	0.00000	-0.01135
18 Ar 1 DXZ	0.02735	0.00000	0.00000	0.00000	0.03791
19 Ar 1 DYZ	-0.00850	0.00000	0.00000	0.00000	-0.01178

MO:	11	12	13	14	15
Eigenvalues:	0.43385	0.48053	0.48053	0.67295	0.69095
	A	A	A	A	A
1 Ar 1 S	0.00000	0.00000	0.00000	-0.00558	0.00000
2 Ar 1 S	0.00000	0.00000	0.00000	0.03461	0.00000
3 Ar 1 PX	0.21514	0.22660	0.07046	0.00000	0.00000
4 Ar 1 PY	-0.06686	-0.03186	0.31408	0.00000	0.00000
5 Ar 1 PZ	0.22328	-0.22788	0.02616	0.00000	0.00000
6 Ar 1 S	0.00000	0.00000	0.00000	-0.10294	0.00000
7 Ar 1 PX	-0.76862	-0.80550	-0.25047	0.00000	0.00000
8 Ar 1 PY	0.23887	0.11325	-1.11645	0.00000	0.00000
9 Ar 1 PZ	-0.79769	0.81005	-0.09298	0.00000	0.00000
10 Ar 1 S	0.00000	0.00000	0.00000	0.06990	0.00000
11 Ar 1 PX	0.84188	0.86566	0.26918	0.00000	0.00000
12 Ar 1 PY	-0.26164	-0.12171	1.19984	0.00000	0.00000
13 Ar 1 PZ	0.87372	-0.87056	0.09992	0.00000	0.00000
14 Ar 1 DXX	0.00000	0.00000	0.00000	0.18700	0.77736
15 Ar 1 DYY	0.00000	0.00000	0.00000	-0.43543	-0.21607
16 Ar 1 DZZ	0.00000	0.00000	0.00000	0.24010	-0.56128
17 Ar 1 DXY	0.00000	0.00000	0.00000	-0.24724	0.26193
18 Ar 1 DXZ	0.00000	0.00000	0.00000	0.82565	0.15353
19 Ar 1 DYZ	0.00000	0.00000	0.00000	-0.25659	0.51363

MO:	16	17	18	19
Eigenvalues:	0.69095	0.75328	0.75328	4.19934
	A	A	A	A
1 Ar 1 S	0.00000	0.00000	0.00000	0.11897
2 Ar 1 S	0.00000	0.00000	0.00000	-1.52996
3 Ar 1 PX	0.00000	0.00000	0.00000	0.00000
4 Ar 1 PY	0.00000	0.00000	0.00000	0.00000
5 Ar 1 PZ	0.00000	0.00000	0.00000	0.00000

6	Ar	1 S	0.00000	0.00000	0.00000	4.34567
7	Ar	1 PX	0.00000	0.00000	0.00000	0.00000
8	Ar	1 PY	0.00000	0.00000	0.00000	0.00000
9	Ar	1 PZ	0.00000	0.00000	0.00000	0.00000
10	Ar	1 S	0.00000	0.00000	0.00000	0.88382
11	Ar	1 PX	0.00000	0.00000	0.00000	0.00000
12	Ar	1 PY	0.00000	0.00000	0.00000	0.00000
13	Ar	1 PZ	0.00000	0.00000	0.00000	0.00000
14	Ar	1 DXX	-0.37541	-0.44664	-0.13846	-2.12006
15	Ar	1 DYY	-0.28406	0.82340	-0.08274	-2.12216
16	Ar	1 DZZ	0.65947	-0.37676	0.22121	-2.11988
17	Ar	1 DXY	0.59508	0.07188	-0.71469	-0.00084
18	Ar	1 DXZ	0.14193	0.51846	-0.05996	0.00280
19	Ar	1 DYZ	0.43366	0.21546	0.66004	-0.00087

Beta Spin Molecular Orbital Coefficients

MO:			1	2	3	4	5
Eigenvalues:			-118.43804	-12.79513	-10.04172	-10.04172	-10.01912
			A	A	A	A	A
1	Ar	1 S	0.98408	0.30620	0.00000	0.00000	0.00000
2	Ar	1 S	0.07593	-0.92453	0.00000	0.00000	0.00000
3	Ar	1 PX	0.00000	0.00000	-0.11015	-0.70832	0.66067
4	Ar	1 PY	0.00000	0.00000	-0.95261	-0.04396	-0.20532
5	Ar	1 PZ	0.00000	0.00000	-0.17913	0.66935	0.68566
6	Ar	1 S	-0.08044	-0.29639	0.00000	0.00000	0.00000
7	Ar	1 PX	0.00000	0.00000	-0.00832	-0.05350	0.05290
8	Ar	1 PY	0.00000	0.00000	-0.07195	-0.00332	-0.01644
9	Ar	1 PZ	0.00000	0.00000	-0.01353	0.05055	0.05490
10	Ar	1 S	-0.00716	0.00802	0.00000	0.00000	0.00000
11	Ar	1 PX	0.00000	0.00000	0.00236	0.01519	-0.01532
12	Ar	1 PY	0.00000	0.00000	0.02043	0.00094	0.00476
13	Ar	1 PZ	0.00000	0.00000	0.00384	-0.01435	-0.01590
14	Ar	1 DXX	0.03180	0.08252	0.00000	0.00000	0.00000
15	Ar	1 DYY	0.03179	0.08229	0.00000	0.00000	0.00000
16	Ar	1 DZZ	0.03180	0.08254	0.00000	0.00000	0.00000
17	Ar	1 DXY	-0.00001	-0.00009	0.00000	0.00000	0.00000
18	Ar	1 DXZ	0.00002	0.00031	0.00000	0.00000	0.00000
19	Ar	1 DYZ	-0.00001	-0.00010	0.00000	0.00000	0.00000

MO:			6	7	8	9	10
Eigenvalues:			-1.64250	-1.01429	-1.01429	-0.49690	0.33088
			A	A	A	A	A
1	Ar	1 S	0.08555	0.00000	0.00000	0.00000	0.05674
2	Ar	1 S	-0.50113	0.00000	0.00000	0.00000	-0.29628
3	Ar	1 PX	0.00000	-0.23357	-0.00197	-0.19198	0.00000
4	Ar	1 PY	0.00000	-0.05928	-0.30503	0.05966	0.00000
5	Ar	1 PZ	0.00000	0.20731	-0.08944	-0.19924	0.00000
6	Ar	1 S	0.66989	0.00000	0.00000	0.00000	1.42248
7	Ar	1 PX	0.00000	0.53840	0.00455	0.40947	0.00000
8	Ar	1 PY	0.00000	0.13664	0.70311	-0.12726	0.00000
9	Ar	1 PZ	0.00000	-0.47786	0.20617	0.42496	0.00000
10	Ar	1 S	0.39595	0.00000	0.00000	0.00000	-1.85789
11	Ar	1 PX	0.00000	0.29811	0.00252	0.36374	0.00000
12	Ar	1 PY	0.00000	0.07566	0.38931	-0.11304	0.00000
13	Ar	1 PZ	0.00000	-0.26459	0.11415	0.37749	0.00000
14	Ar	1 DXX	0.02092	0.00000	0.00000	0.00000	0.19993

```
15 Ar  1 DYY       0.04375    0.00000    0.00000    0.00000    0.20520
16 Ar  1 DZZ       0.01897    0.00000    0.00000    0.00000    0.19948
17 Ar  1 DXY       0.00907    0.00000    0.00000    0.00000    0.00209
18 Ar  1 DXZ      -0.03029    0.00000    0.00000    0.00000   -0.00698
19 Ar  1 DYZ       0.00941    0.00000    0.00000    0.00000    0.00217

MO:                  11         12         13         14         15

Eigenvalues:       0.49030    0.49030    0.53490    0.76446    0.76446

                      A          A          A          A          A
 1 Ar  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
 2 Ar  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
 3 Ar  1 PX        0.23746    0.02797    0.24430    0.00000    0.00000
 4 Ar  1 PY        0.02641    0.31698   -0.07592    0.00000    0.00000
 5 Ar  1 PZ       -0.22090    0.06797    0.25354    0.00000    0.00000
 6 Ar  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
 7 Ar  1 PX       -0.84194   -0.09918   -0.83150    0.00000    0.00000
 8 Ar  1 PY       -0.09364   -1.12390    0.25841    0.00000    0.00000
 9 Ar  1 PZ        0.78322   -0.24099   -0.86295    0.00000    0.00000
10 Ar  1 S         0.00000    0.00000    0.00000    0.00000    0.00000
11 Ar  1 PX        0.89804    0.10579    0.80005    0.00000    0.00000
12 Ar  1 PY        0.09988    1.19879   -0.24864    0.00000    0.00000
13 Ar  1 PZ       -0.83540    0.25705    0.83030    0.00000    0.00000
14 Ar  1 DXX       0.00000    0.00000    0.00000   -0.43028   -0.18308
15 Ar  1 DYY       0.00000    0.00000    0.00000    0.82754    0.00125
16 Ar  1 DZZ       0.00000    0.00000    0.00000   -0.39727    0.18183
17 Ar  1 DXY       0.00000    0.00000    0.00000    0.14404   -0.70371
18 Ar  1 DXZ       0.00000    0.00000    0.00000    0.52187   -0.00704
19 Ar  1 DYZ       0.00000    0.00000    0.00000    0.14736    0.67850

MO:                  16         17         18         19

Eigenvalues:       0.80335    0.80335    0.81883    4.22749

                      A          A          A          A
 1 Ar  1 S         0.00000    0.00000    0.00340    0.11908
 2 Ar  1 S         0.00000    0.00000   -0.01953   -1.53057
 3 Ar  1 PX        0.00000    0.00000    0.00000    0.00000
 4 Ar  1 PY        0.00000    0.00000    0.00000    0.00000
 5 Ar  1 PZ        0.00000    0.00000    0.00000    0.00000
 6 Ar  1 S         0.00000    0.00000    0.03385    4.34937
 7 Ar  1 PX        0.00000    0.00000    0.00000    0.00000
 8 Ar  1 PY        0.00000    0.00000    0.00000    0.00000
 9 Ar  1 PZ        0.00000    0.00000    0.00000    0.00000
10 Ar  1 S         0.00000    0.00000   -0.00176    0.87754
11 Ar  1 PX        0.00000    0.00000    0.00000    0.00000
12 Ar  1 PY        0.00000    0.00000    0.00000    0.00000
13 Ar  1 PZ        0.00000    0.00000    0.00000    0.00000
14 Ar  1 DXX      -0.84073   -0.19593    0.19402   -2.11998
15 Ar  1 DYY      -0.01020    0.35676   -0.42897   -2.12038
16 Ar  1 DZZ       0.85093   -0.16083    0.24717   -2.11994
17 Ar  1 DXY       0.16979   -0.62761   -0.24747   -0.00016
18 Ar  1 DXZ      -0.03037   -0.20687    0.82639    0.00054
19 Ar  1 DYZ      -0.12746   -0.66002   -0.25683   -0.00017

  ** Archive file written to unit 12 **

Total Cpu time:        0 mins.  1.92 secs.
Total Wall time:       0 mins.  2.49 secs.
```

```
  Calculation finished: Fri Sep 18 13:40:09 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:40:52 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   6
     1 S shells
     4 SP shells
     1 6D shells
  Number of basis functions:  23
  Number of electrons:  19
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    K  K1           0.0000000     0.3727813     1.3078904

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to -.45E-09 in   9 cycles  <S**2> = 0.7501

  E(HF)  =    -596.1532433 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:    -132.61956  -14.41784  -11.43261  -11.43261  -11.43261

                        A         A         A         A         A
   1 K   1 S        -0.98642   -0.30412    0.00000    0.00000    0.00000
   2 K   1 S        -0.04951    1.01728    0.00000    0.00000    0.00000
   3 K   1 PX        0.00000    0.00000   -0.38168   -0.01402   -0.91186
   4 K   1 PY        0.00000    0.00000    0.86865   -0.30663   -0.35888
   5 K   1 PZ        0.00000    0.00000   -0.27773   -0.93976    0.13070
   6 K   1 S         0.01022    0.04591    0.00000    0.00000    0.00000
   7 K   1 PX        0.00000    0.00000   -0.01476   -0.00054   -0.03526
   8 K   1 PY        0.00000    0.00000    0.03359   -0.01186   -0.01388
   9 K   1 PZ        0.00000    0.00000   -0.01074   -0.03634    0.00505
  10 K   1 S        -0.00310   -0.00769    0.00000    0.00000    0.00000
  11 K   1 PX        0.00000    0.00000    0.00339    0.00012    0.00809
  12 K   1 PY        0.00000    0.00000   -0.00771    0.00272    0.00318
  13 K   1 PZ        0.00000    0.00000    0.00246    0.00834   -0.00116
  14 K   1 S         0.00129    0.00408    0.00000    0.00000    0.00000
  15 K   1 PX        0.00000    0.00000   -0.00194   -0.00007   -0.00463
  16 K   1 PY        0.00000    0.00000    0.00442   -0.00156   -0.00182
  17 K   1 PZ        0.00000    0.00000   -0.00141   -0.00478    0.00066
  18 K   1 DXX       0.00004   -0.00091    0.00000    0.00000    0.00000
  19 K   1 DYY       0.00004   -0.00091    0.00000    0.00000    0.00000
```

20 K	1 DZZ	0.00004	-0.00091	0.00000	0.00000	0.00000
21 K	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 K	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23 K	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		6	7	8	9	10
Eigenvalues:		-1.74746	-0.94903	-0.94903	-0.94903	-0.14674
		A	A	A	A	A
1 K	1 S	0.10011	0.00000	0.00000	0.00000	-0.01939
2 K	1 S	-0.38378	0.00000	0.00000	0.00000	0.06675
3 K	1 PX	0.00000	0.26997	-0.06346	0.17183	0.00000
4 K	1 PY	0.00000	-0.18116	-0.13776	0.23375	0.00000
5 K	1 PZ	0.00000	0.02709	-0.28885	-0.14923	0.00000
6 K	1 S	1.04819	0.00000	0.00000	0.00000	-0.26380
7 K	1 PX	0.00000	-0.85055	0.19993	-0.54136	0.00000
8 K	1 PY	0.00000	0.57076	0.43401	-0.73645	0.00000
9 K	1 PZ	0.00000	-0.08534	0.91003	0.47016	0.00000
10 K	1 S	-0.04911	0.00000	0.00000	0.00000	0.68850
11 K	1 PX	0.00000	-0.05950	0.01399	-0.03787	0.00000
12 K	1 PY	0.00000	0.03993	0.03036	-0.05152	0.00000
13 K	1 PZ	0.00000	-0.00597	0.06366	0.03289	0.00000
14 K	1 S	0.01363	0.00000	0.00000	0.00000	0.42566
15 K	1 PX	0.00000	0.02672	-0.00628	0.01701	0.00000
16 K	1 PY	0.00000	-0.01793	-0.01363	0.02313	0.00000
17 K	1 PZ	0.00000	0.00268	-0.02859	-0.01477	0.00000
18 K	1 DXX	0.02368	0.00000	0.00000	0.00000	-0.02773
19 K	1 DYY	0.02368	0.00000	0.00000	0.00000	-0.02773
20 K	1 DZZ	0.02368	0.00000	0.00000	0.00000	-0.02773
21 K	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 K	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23 K	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.01451	0.01451	0.01451	0.05594	0.10388
		A	A	A	A	A
1 K	1 S	0.00000	0.00000	0.00000	0.00784	0.00000
2 K	1 S	0.00000	0.00000	0.00000	-0.06966	0.00000
3 K	1 PX	-0.02302	-0.01252	-0.01899	0.00000	0.02294
4 K	1 PY	0.02233	-0.00730	-0.02226	0.00000	0.07164
5 K	1 PZ	0.00433	-0.02894	0.01383	0.00000	0.02232
6 K	1 S	0.00000	0.00000	0.00000	-0.04999	0.00000
7 K	1 PX	0.08311	0.04521	0.06854	0.00000	-0.08601
8 K	1 PY	-0.08061	0.02634	0.08036	0.00000	-0.26863
9 K	1 PZ	-0.01565	0.10446	-0.04993	0.00000	-0.08369
10 K	1 S	0.00000	0.00000	0.00000	-4.47377	0.00000
11 K	1 PX	-0.04659	-0.02535	-0.03843	0.00000	0.48811
12 K	1 PY	0.04519	-0.01476	-0.04506	0.00000	1.52452
13 K	1 PZ	0.00877	-0.05856	0.02799	0.00000	0.47498
14 K	1 S	0.00000	0.00000	0.00000	2.88220	0.00000
15 K	1 PX	-0.67652	-0.36802	-0.55796	0.00000	-0.39104
16 K	1 PY	0.65615	-0.21438	-0.65418	0.00000	-1.22134
17 K	1 PZ	0.12738	-0.85032	0.40641	0.00000	-0.38052
18 K	1 DXX	0.00000	0.00000	0.00000	0.80077	0.00000
19 K	1 DYY	0.00000	0.00000	0.00000	0.80077	0.00000
20 K	1 DZZ	0.00000	0.00000	0.00000	0.80077	0.00000
21 K	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 K	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

23 K	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		16	17	18	19	20
Eigenvalues:		0.10388	0.10388	0.22737	0.22737	0.22737
		A	A	A	A	A
1 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 K	1 PX	-0.02378	0.07117	0.00000	0.00000	0.00000
4 K	1 PY	-0.01519	-0.02817	0.00000	0.00000	0.00000
5 K	1 PZ	0.07321	0.01727	0.00000	0.00000	0.00000
6 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 K	1 PX	0.08918	-0.26686	0.00000	0.00000	0.00000
8 K	1 PY	0.05698	0.10562	0.00000	0.00000	0.00000
9 K	1 PZ	-0.27452	-0.06477	0.00000	0.00000	0.00000
10 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 K	1 PX	-0.50614	1.51446	0.00000	0.00000	0.00000
12 K	1 PY	-0.32335	-0.59942	0.00000	0.00000	0.00000
13 K	1 PZ	1.55798	0.36760	0.00000	0.00000	0.00000
14 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
15 K	1 PX	0.40548	-1.21328	0.00000	0.00000	0.00000
16 K	1 PY	0.25904	0.48021	0.00000	0.00000	0.00000
17 K	1 PZ	-1.24814	-0.29449	0.00000	0.00000	0.00000
18 K	1 DXX	0.00000	0.00000	-0.13150	0.27310	0.87504
19 K	1 DYY	0.00000	0.00000	-0.69950	-0.11983	-0.69323
20 K	1 DZZ	0.00000	0.00000	0.83100	-0.15326	-0.18181
21 K	1 DXY	0.00000	0.00000	-0.44860	-0.08295	0.31682
22 K	1 DXZ	0.00000	0.00000	0.02430	0.36515	-0.09029
23 K	1 DYZ	0.00000	0.00000	0.00777	0.88591	-0.19644

MO:		21	22	23
Eigenvalues:		0.22737	0.22737	0.30817
		A	A	A
1 K	1 S	0.00000	0.00000	-0.00501
2 K	1 S	0.00000	0.00000	-0.00379
3 K	1 PX	0.00000	0.00000	0.00000
4 K	1 PY	0.00000	0.00000	0.00000
5 K	1 PZ	0.00000	0.00000	0.00000
6 K	1 S	0.00000	0.00000	-0.12429
7 K	1 PX	0.00000	0.00000	0.00000
8 K	1 PY	0.00000	0.00000	0.00000
9 K	1 PZ	0.00000	0.00000	0.00000
10 K	1 S	0.00000	0.00000	-8.30179
11 K	1 PX	0.00000	0.00000	0.00000
12 K	1 PY	0.00000	0.00000	0.00000
13 K	1 PZ	0.00000	0.00000	0.00000
14 K	1 S	0.00000	0.00000	2.37070
15 K	1 PX	0.00000	0.00000	0.00000
16 K	1 PY	0.00000	0.00000	0.00000
17 K	1 PZ	0.00000	0.00000	0.00000
18 K	1 DXX	0.37453	0.04638	2.90395
19 K	1 DYY	0.12506	0.01114	2.90395
20 K	1 DZZ	-0.49959	-0.05752	2.90395
21 K	1 DXY	-0.82043	-0.13561	0.00000
22 K	1 DXZ	0.06762	-0.92377	0.00000
23 K	1 DYZ	-0.22800	0.35289	0.00000

Beta Spin Molecular Orbital Coefficients

MO:		1	2	3	4	5
Eigenvalues:		-132.61869	-14.41620	-11.43212	-11.43212	-11.43212
		A	A	A	A	A
1 K	1 S	-0.98642	-0.30411	0.00000	0.00000	0.00000
2 K	1 S	-0.04952	1.01725	0.00000	0.00000	0.00000
3 K	1 PX	0.00000	0.00000	0.97379	0.08816	0.14607
4 K	1 PY	0.00000	0.00000	0.14377	0.03170	-0.97760
5 K	1 PZ	0.00000	0.00000	-0.09186	0.98417	0.01841
6 K	1 S	0.01022	0.04599	0.00000	0.00000	0.00000
7 K	1 PX	0.00000	0.00000	0.03763	0.00341	0.00564
8 K	1 PY	0.00000	0.00000	0.00556	0.00123	-0.03778
9 K	1 PZ	0.00000	0.00000	-0.00355	0.03803	0.00071
10 K	1 S	-0.00310	-0.00770	0.00000	0.00000	0.00000
11 K	1 PX	0.00000	0.00000	-0.00861	-0.00078	-0.00129
12 K	1 PY	0.00000	0.00000	-0.00127	-0.00028	0.00864
13 K	1 PZ	0.00000	0.00000	0.00081	-0.00870	-0.00016
14 K	1 S	0.00129	0.00409	0.00000	0.00000	0.00000
15 K	1 PX	0.00000	0.00000	0.00494	0.00045	0.00074
16 K	1 PY	0.00000	0.00000	0.00073	0.00016	-0.00496
17 K	1 PZ	0.00000	0.00000	-0.00047	0.00499	0.00009
18 K	1 DXX	0.00004	-0.00092	0.00000	0.00000	0.00000
19 K	1 DYY	0.00004	-0.00092	0.00000	0.00000	0.00000
20 K	1 DZZ	0.00004	-0.00092	0.00000	0.00000	0.00000
21 K	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 K	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23 K	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		6	7	8	9	10
Eigenvalues:		-1.74263	-0.94712	-0.94712	-0.94712	0.01099
		A	A	A	A	A
1 K	1 S	0.10012	0.00000	0.00000	0.00000	0.01388
2 K	1 S	-0.38378	0.00000	0.00000	0.00000	-0.02985
3 K	1 PX	0.00000	0.27051	-0.09910	0.15425	0.00000
4 K	1 PY	0.00000	-0.18132	-0.10392	0.25122	0.00000
5 K	1 PZ	0.00000	0.02713	0.29354	0.14101	0.00000
6 K	1 S	1.04801	0.00000	0.00000	0.00000	0.25514
7 K	1 PX	0.00000	-0.85254	0.31233	-0.48614	0.00000
8 K	1 PY	0.00000	0.57146	0.32752	-0.79175	0.00000
9 K	1 PZ	0.00000	-0.08551	-0.92514	-0.44442	0.00000
10 K	1 S	-0.04833	0.00000	0.00000	0.00000	1.05356
11 K	1 PX	0.00000	-0.05204	0.01907	-0.02968	0.00000
12 K	1 PY	0.00000	0.03488	0.01999	-0.04833	0.00000
13 K	1 PZ	0.00000	-0.00522	-0.05648	-0.02713	0.00000
14 K	1 S	0.01315	0.00000	0.00000	0.00000	-1.56128
15 K	1 PX	0.00000	0.02455	-0.00899	0.01400	0.00000
16 K	1 PY	0.00000	-0.01645	-0.00943	0.02280	0.00000
17 K	1 PZ	0.00000	0.00246	0.02664	0.01280	0.00000
18 K	1 DXX	0.02385	0.00000	0.00000	0.00000	-0.22622
19 K	1 DYY	0.02385	0.00000	0.00000	0.00000	-0.22622
20 K	1 DZZ	0.02385	0.00000	0.00000	0.00000	-0.22622
21 K	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 K	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23 K	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15

Eigenvalues:		0.03254	0.03254	0.03254	0.07975	0.12884
		A	A	A	A	A
1 K	1 S	0.00000	0.00000	0.00000	-0.01522	0.00000
2 K	1 S	0.00000	0.00000	0.00000	0.09208	0.00000
3 K	1 PX	-0.01259	-0.00161	-0.00903	0.00000	0.02749
4 K	1 PY	0.00906	0.00011	-0.01266	0.00000	-0.07581
5 K	1 PZ	-0.00137	0.01549	-0.00085	0.00000	0.00974
6 K	1 S	0.00000	0.00000	0.00000	-0.06258	0.00000
7 K	1 PX	0.04420	0.00564	0.03169	0.00000	-0.10320
8 K	1 PY	-0.03183	-0.00038	0.04446	0.00000	0.28464
9 K	1 PZ	0.00481	-0.05439	0.00297	0.00000	-0.03656
10 K	1 S	0.00000	0.00000	0.00000	4.83743	0.00000
11 K	1 PX	0.20651	0.02635	0.14805	0.00000	0.55893
12 K	1 PY	-0.14869	-0.00180	0.20772	0.00000	-1.54165
13 K	1 PZ	0.02247	-0.25409	0.01389	0.00000	0.19800
14 K	1 S	0.00000	0.00000	0.00000	-2.55294	0.00000
15 K	1 PX	-0.96167	-0.12272	-0.68946	0.00000	-0.38265
16 K	1 PY	0.69244	0.00836	-0.96731	0.00000	1.05544
17 K	1 PZ	-0.10463	1.18325	-0.06467	0.00000	-0.13556
18 K	1 DXX	0.00000	0.00000	0.00000	-0.91293	0.00000
19 K	1 DYY	0.00000	0.00000	0.00000	-0.91293	0.00000
20 K	1 DZZ	0.00000	0.00000	0.00000	-0.91293	0.00000
21 K	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 K	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23 K	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		16	17	18	19	20
Eigenvalues:		0.12884	0.12884	0.24671	0.24671	0.24671
		A	A	A	A	A
1 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 K	1 PX	-0.03443	-0.06824	0.00000	0.00000	0.00000
4 K	1 PY	-0.02152	-0.01968	0.00000	0.00000	0.00000
5 K	1 PZ	-0.07035	0.03942	0.00000	0.00000	0.00000
6 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 K	1 PX	0.12928	0.25621	0.00000	0.00000	0.00000
8 K	1 PY	0.08080	0.07388	0.00000	0.00000	0.00000
9 K	1 PZ	0.26413	-0.14801	0.00000	0.00000	0.00000
10 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 K	1 PX	-0.70022	-1.38765	0.00000	0.00000	0.00000
12 K	1 PY	-0.43760	-0.40014	0.00000	0.00000	0.00000
13 K	1 PZ	-1.43055	0.80162	0.00000	0.00000	0.00000
14 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
15 K	1 PX	0.47938	0.95001	0.00000	0.00000	0.00000
16 K	1 PY	0.29959	0.27394	0.00000	0.00000	0.00000
17 K	1 PZ	0.97939	-0.54880	0.00000	0.00000	0.00000
18 K	1 DXX	0.00000	0.00000	0.88655	0.46068	-0.04138
19 K	1 DYY	0.00000	0.00000	-0.84388	0.53440	-0.04770
20 K	1 DZZ	0.00000	0.00000	-0.04267	-0.99508	0.08908
21 K	1 DXY	0.00000	0.00000	0.00664	0.01423	0.07688
22 K	1 DXZ	0.00000	0.00000	-0.00152	0.02339	0.25467
23 K	1 DYZ	0.00000	0.00000	0.00003	0.08516	0.95983

MO:		21	22	23
Eigenvalues:		0.24671	0.24671	0.31966
		A	A	A

```
  1 K   1 S         0.00000    0.00000    0.00647
  2 K   1 S         0.00000    0.00000   -0.00306
  3 K   1 PX        0.00000    0.00000    0.00000
  4 K   1 PY        0.00000    0.00000    0.00000
  5 K   1 PZ        0.00000    0.00000    0.00000
  6 K   1 S         0.00000    0.00000    0.13740
  7 K   1 PX        0.00000    0.00000    0.00000
  8 K   1 PY        0.00000    0.00000    0.00000
  9 K   1 PZ        0.00000    0.00000    0.00000
 10 K   1 S         0.00000    0.00000    8.05592
 11 K   1 PX        0.00000    0.00000    0.00000
 12 K   1 PY        0.00000    0.00000    0.00000
 13 K   1 PZ        0.00000    0.00000    0.00000
 14 K   1 S         0.00000    0.00000   -2.27011
 15 K   1 PX        0.00000    0.00000    0.00000
 16 K   1 PY        0.00000    0.00000    0.00000
 17 K   1 PZ        0.00000    0.00000    0.00000
 18 K   1 DXX       0.00932    0.00069   -2.86187
 19 K   1 DYY      -0.00194    0.00134   -2.86187
 20 K   1 DZZ      -0.00738   -0.00203   -2.86187
 21 K   1 DXY      -0.98145   -0.17491    0.00000
 22 K   1 DXZ       0.18924   -0.94804    0.00000
 23 K   1 DYZ       0.02906    0.26574    0.00000

   ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  3.05 secs.
  Total Wall time:       0 mins.  3.57 secs.

  Calculation finished: Fri Sep 18 13:40:56 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.08 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:42:28 1998

  Run type: Single point energy
  Model: RHF/3-21G(*)
  Number of shells:   6
     1 S shells
     4 SP shells
     1 6D shells
  Number of basis functions:  23
  Number of electrons:  20
  Use of molecular symmetry disabled
  Molecular charge:   0
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Ca Ca1          0.0000000     2.0502961    -2.0786987

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  RHF direct SCF procedure requested

  Energy converged to -.40E-11 in  13 cycles

  E(HF)  =    -673.4185120 a.u.

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:    -148.37255  -16.75401  -13.54347  -13.54347  -13.54347

                        A         A         A         A         A
   1 Ca  1 S         0.98577   0.30637   0.00000   0.00000   0.00000
   2 Ca  1 S         0.05167  -1.01371   0.00000   0.00000   0.00000
   3 Ca  1 PX        0.00000   0.00000   0.97963   0.12051  -0.02647
   4 Ca  1 PY        0.00000   0.00000   0.07091  -0.37649   0.91001
   5 Ca  1 PZ        0.00000   0.00000  -0.10097   0.90478   0.38220
   6 Ca  1 S        -0.01415  -0.05528   0.00000   0.00000   0.00000
   7 Ca  1 PX        0.00000   0.00000   0.03953   0.00486  -0.00107
   8 Ca  1 PY        0.00000   0.00000   0.00286  -0.01519   0.03672
   9 Ca  1 PZ        0.00000   0.00000  -0.00407   0.03651   0.01542
  10 Ca  1 S         0.02954   0.07627   0.00000   0.00000   0.00000
  11 Ca  1 PX        0.00000   0.00000  -0.00992  -0.00122   0.00027
  12 Ca  1 PY        0.00000   0.00000  -0.00072   0.00381  -0.00922
  13 Ca  1 PZ        0.00000   0.00000   0.00102  -0.00916  -0.00387
  14 Ca  1 S        -0.00027  -0.00232   0.00000   0.00000   0.00000
  15 Ca  1 PX        0.00000   0.00000   0.00551   0.00068  -0.00015
  16 Ca  1 PY        0.00000   0.00000   0.00040  -0.00212   0.00512
  17 Ca  1 PZ        0.00000   0.00000  -0.00057   0.00509   0.00215
  18 Ca  1 DXX      -0.01188  -0.02966   0.00000   0.00000   0.00000
  19 Ca  1 DYY      -0.01188  -0.02966   0.00000   0.00000   0.00000
```

20 Ca	1 DZZ	-0.01188	-0.02966	0.00000	0.00000	0.00000
21 Ca	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 Ca	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23 Ca	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		6	7	8	9	10
Eigenvalues:		-2.24619	-1.33738	-1.33738	-1.33738	-0.19500
		A	A	A	A	A
1 Ca	1 S	0.10611	0.00000	0.00000	0.00000	0.02536
2 Ca	1 S	-0.40365	0.00000	0.00000	0.00000	-0.09245
3 Ca	1 PX	0.00000	0.21830	0.27352	-0.00279	0.00000
4 Ca	1 PY	0.00000	-0.26357	0.20938	-0.09570	0.00000
5 Ca	1 PZ	0.00000	-0.07313	0.06180	0.33661	0.00000
6 Ca	1 S	1.05482	0.00000	0.00000	0.00000	0.31569
7 Ca	1 PX	0.00000	-0.64554	-0.80884	0.00826	0.00000
8 Ca	1 PY	0.00000	0.77944	-0.61919	0.28300	0.00000
9 Ca	1 PZ	0.00000	0.21624	-0.18275	-0.99541	0.00000
10 Ca	1 S	0.01567	0.00000	0.00000	0.00000	-0.66710
11 Ca	1 PX	0.00000	-0.03667	-0.04594	0.00047	0.00000
12 Ca	1 PY	0.00000	0.04427	-0.03517	0.01608	0.00000
13 Ca	1 PZ	0.00000	0.01228	-0.01038	-0.05654	0.00000
14 Ca	1 S	-0.00950	0.00000	0.00000	0.00000	-0.40793
15 Ca	1 PX	0.00000	0.01492	0.01869	-0.00019	0.00000
16 Ca	1 PY	0.00000	-0.01801	0.01431	-0.00654	0.00000
17 Ca	1 PZ	0.00000	-0.00500	0.00422	0.02300	0.00000
18 Ca	1 DXX	0.00365	0.00000	0.00000	0.00000	0.00205
19 Ca	1 DYY	0.00365	0.00000	0.00000	0.00000	0.00205
20 Ca	1 DZZ	0.00365	0.00000	0.00000	0.00000	0.00205
21 Ca	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 Ca	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23 Ca	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		0.02213	0.02213	0.02213	0.10012	0.14262
		A	A	A	A	A
1 Ca	1 S	0.00000	0.00000	0.00000	0.01158	0.00000
2 Ca	1 S	0.00000	0.00000	0.00000	-0.09517	0.00000
3 Ca	1 PX	0.03027	0.02186	-0.02035	0.00000	0.02403
4 Ca	1 PY	-0.02173	0.03600	0.00634	0.00000	-0.08619
5 Ca	1 PZ	-0.02049	-0.00589	-0.03680	0.00000	-0.01988
6 Ca	1 S	0.00000	0.00000	0.00000	-0.03401	0.00000
7 Ca	1 PX	-0.10517	-0.07596	0.07072	0.00000	-0.08711
8 Ca	1 PY	0.07552	-0.12508	-0.02203	0.00000	0.31245
9 Ca	1 PZ	0.07119	0.02046	0.12785	0.00000	0.07208
10 Ca	1 S	0.00000	0.00000	0.00000	-1.63269	0.00000
11 Ca	1 PX	0.09990	0.07215	-0.06717	0.00000	0.43475
12 Ca	1 PY	-0.07173	0.11880	0.02093	0.00000	-1.55928
13 Ca	1 PZ	-0.06762	-0.01943	-0.12144	0.00000	-0.35970
14 Ca	1 S	0.00000	0.00000	0.00000	2.10779	0.00000
15 Ca	1 PX	0.63579	0.45918	-0.42753	0.00000	-0.35450
16 Ca	1 PY	-0.45652	0.75612	0.13320	0.00000	1.27146
17 Ca	1 PZ	-0.43037	-0.12369	-0.77288	0.00000	0.29331
18 Ca	1 DXX	0.00000	0.00000	0.00000	-0.18135	0.00000
19 Ca	1 DYY	0.00000	0.00000	0.00000	-0.18135	0.00000
20 Ca	1 DZZ	0.00000	0.00000	0.00000	-0.18135	0.00000
21 Ca	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 Ca	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

23 Ca	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		16	17	18	19	20
Eigenvalues:		0.14262	0.14262	0.20849	0.20849	0.20849
		A	A	A	A	A
1 Ca	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 Ca	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 Ca	1 PX	-0.06279	0.06231	0.00000	0.00000	0.00000
4 Ca	1 PY	-0.03114	0.00187	0.00000	0.00000	0.00000
5 Ca	1 PZ	0.05908	0.06721	0.00000	0.00000	0.00000
6 Ca	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 Ca	1 PX	0.22761	-0.22586	0.00000	0.00000	0.00000
8 Ca	1 PY	0.11286	-0.00678	0.00000	0.00000	0.00000
9 Ca	1 PZ	-0.21416	-0.24362	0.00000	0.00000	0.00000
10 Ca	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 Ca	1 PX	-1.13588	1.12718	0.00000	0.00000	0.00000
12 Ca	1 PY	-0.56325	0.03381	0.00000	0.00000	0.00000
13 Ca	1 PZ	1.06878	1.21577	0.00000	0.00000	0.00000
14 Ca	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
15 Ca	1 PX	0.92621	-0.91912	0.00000	0.00000	0.00000
16 Ca	1 PY	0.45928	-0.02757	0.00000	0.00000	0.00000
17 Ca	1 PZ	-0.87149	-0.99135	0.00000	0.00000	0.00000
18 Ca	1 DXX	0.00000	0.00000	-0.00002	0.26088	-0.54823
19 Ca	1 DYY	0.00000	0.00000	-0.00002	0.24900	0.55683
20 Ca	1 DZZ	0.00000	0.00000	0.00004	-0.50988	-0.00860
21 Ca	1 DXY	0.00000	0.00000	0.79372	-0.31751	-0.37227
22 Ca	1 DXZ	0.00000	0.00000	0.48871	0.73999	0.11206
23 Ca	1 DYZ	0.00000	0.00000	0.36217	-0.30261	0.66463

MO:		21	22	23
Eigenvalues:		0.20849	0.20849	0.65804
		A	A	A
1 Ca	1 S	0.00000	0.00000	-0.05185
2 Ca	1 S	0.00000	0.00000	0.21729
3 Ca	1 PX	0.00000	0.00000	0.00000
4 Ca	1 PY	0.00000	0.00000	0.00000
5 Ca	1 PZ	0.00000	0.00000	0.00000
6 Ca	1 S	0.00000	0.00000	-0.61190
7 Ca	1 PX	0.00000	0.00000	0.00000
8 Ca	1 PY	0.00000	0.00000	0.00000
9 Ca	1 PZ	0.00000	0.00000	0.00000
10 Ca	1 S	0.00000	0.00000	5.17118
11 Ca	1 PX	0.00000	0.00000	0.00000
12 Ca	1 PY	0.00000	0.00000	0.00000
13 Ca	1 PZ	0.00000	0.00000	0.00000
14 Ca	1 S	0.00000	0.00000	0.31059
15 Ca	1 PX	0.00000	0.00000	0.00000
16 Ca	1 PY	0.00000	0.00000	0.00000
17 Ca	1 PZ	0.00000	0.00000	0.00000
18 Ca	1 DXX	-0.66162	-0.44005	-2.41551
19 Ca	1 DYY	0.67191	-0.42009	-2.41551
20 Ca	1 DZZ	-0.01029	0.86014	-2.41551
21 Ca	1 DXY	0.30847	-0.18829	0.00000
22 Ca	1 DXZ	-0.09283	0.43864	0.00000
23 Ca	1 DYZ	-0.55077	-0.17935	0.00000

** Archive file written to unit 12 **

```
  Total Cpu time:        0 mins.  4.14 secs.
  Total Wall time:       0 mins.  4.64 secs.

  Calculation finished: Fri Sep 18 13:42:33 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.06 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:41:23 1998

  Run type: Single point energy
  Model: RHF/3-21G(*)
  Number of shells:   6
     1 S shells
     4 SP shells
     1 6D shells
  Number of basis functions:  23
  Number of electrons:  18
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    K  K1           0.0000000     0.3727813     1.3078904

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  RHF direct SCF procedure requested

  Energy converged to -.60E-09 in   7 cycles

  E(HF)  =    -596.0068253 a.u.

  Closed-Shell Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:    -132.84130  -14.63736  -11.65344  -11.65344  -11.65344

                        A         A         A         A         A
   1 K   1 S        -0.98642   -0.30412    0.00000    0.00000    0.00000
   2 K   1 S        -0.04952    1.01726    0.00000    0.00000    0.00000
   3 K   1 PX        0.00000    0.00000    0.53223   -0.81208   -0.18618
   4 K   1 PY        0.00000    0.00000   -0.22304    0.07398   -0.96031
   5 K   1 PZ        0.00000    0.00000    0.80274    0.55898   -0.14338
   6 K   1 S         0.01022    0.04596    0.00000    0.00000    0.00000
   7 K   1 PX        0.00000    0.00000    0.02054   -0.03134   -0.00719
   8 K   1 PY        0.00000    0.00000   -0.00861    0.00286   -0.03706
   9 K   1 PZ        0.00000    0.00000    0.03098    0.02157   -0.00553
  10 K   1 S        -0.00310   -0.00759    0.00000    0.00000    0.00000
  11 K   1 PX        0.00000    0.00000   -0.00468    0.00714    0.00164
  12 K   1 PY        0.00000    0.00000    0.00196   -0.00065    0.00844
  13 K   1 PZ        0.00000    0.00000   -0.00706   -0.00491    0.00126
  14 K   1 S         0.00129    0.00404    0.00000    0.00000    0.00000
  15 K   1 PX        0.00000    0.00000    0.00268   -0.00409   -0.00094
  16 K   1 PY        0.00000    0.00000   -0.00112    0.00037   -0.00483
  17 K   1 PZ        0.00000    0.00000    0.00404    0.00281   -0.00072
  18 K   1 DXX       0.00004   -0.00095    0.00000    0.00000    0.00000
  19 K   1 DYY       0.00004   -0.00095    0.00000    0.00000    0.00000
```

20 K	1 DZZ	0.00004	-0.00095	0.00000	0.00000	0.00000
21 K	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 K	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23 K	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		6	7	8	9	10
Eigenvalues:		-1.96054	-1.16434	-1.16434	-1.16434	-0.14612
		A	A	A	A	A
1 K	1 S	-0.10013	0.00000	0.00000	0.00000	0.01935
2 K	1 S	0.38383	0.00000	0.00000	0.00000	-0.06647
3 K	1 PX	0.00000	-0.12280	0.27233	-0.13303	0.00000
4 K	1 PY	0.00000	-0.11285	0.09213	0.29277	0.00000
5 K	1 PZ	0.00000	0.28129	0.15585	0.05938	0.00000
6 K	1 S	-1.04826	0.00000	0.00000	0.00000	0.26370
7 K	1 PX	0.00000	0.38713	-0.85852	0.41937	0.00000
8 K	1 PY	0.00000	0.35576	-0.29043	-0.92297	0.00000
9 K	1 PZ	0.00000	-0.88677	-0.49132	-0.18721	0.00000
10 K	1 S	0.04678	0.00000	0.00000	0.00000	-0.68069
11 K	1 PX	0.00000	0.02168	-0.04807	0.02348	0.00000
12 K	1 PY	0.00000	0.01992	-0.01626	-0.05168	0.00000
13 K	1 PZ	0.00000	-0.04965	-0.02751	-0.01048	0.00000
14 K	1 S	-0.01273	0.00000	0.00000	0.00000	-0.43319
15 K	1 PX	0.00000	-0.01006	0.02232	-0.01090	0.00000
16 K	1 PY	0.00000	-0.00925	0.00755	0.02399	0.00000
17 K	1 PZ	0.00000	0.02305	0.01277	0.00487	0.00000
18 K	1 DXX	-0.02290	0.00000	0.00000	0.00000	0.02753
19 K	1 DYY	-0.02290	0.00000	0.00000	0.00000	0.02753
20 K	1 DZZ	-0.02290	0.00000	0.00000	0.00000	0.02753
21 K	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 K	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23 K	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		-0.09531	-0.09531	-0.09531	-0.04627	-0.01763
		A	A	A	A	A
1 K	1 S	0.00000	0.00000	0.00000	0.00828	0.00000
2 K	1 S	0.00000	0.00000	0.00000	-0.06939	0.00000
3 K	1 PX	0.02905	-0.03619	0.00474	0.00000	0.05983
4 K	1 PY	0.03426	0.02912	0.01242	0.00000	0.02780
5 K	1 PZ	-0.01259	-0.00426	0.04471	0.00000	-0.01143
6 K	1 S	0.00000	0.00000	0.00000	-0.03915	0.00000
7 K	1 PX	-0.10716	0.13351	-0.01748	0.00000	-0.22659
8 K	1 PY	-0.12637	-0.10744	-0.04582	0.00000	-0.10526
9 K	1 PZ	0.04646	0.01570	-0.16495	0.00000	0.04330
10 K	1 S	0.00000	0.00000	0.00000	-3.81234	0.00000
11 K	1 PX	0.27333	-0.34052	0.04457	0.00000	1.44130
12 K	1 PY	0.32233	0.27403	0.11687	0.00000	0.66955
13 K	1 PZ	-0.11850	-0.04004	0.42071	0.00000	-0.27543
14 K	1 S	0.00000	0.00000	0.00000	2.68629	0.00000
15 K	1 PX	0.39012	-0.48601	0.06362	0.00000	-1.35571
16 K	1 PY	0.46006	0.39112	0.16681	0.00000	-0.62979
17 K	1 PZ	-0.16913	-0.05715	0.60048	0.00000	0.25907
18 K	1 DXX	0.00000	0.00000	0.00000	0.57104	0.00000
19 K	1 DYY	0.00000	0.00000	0.00000	0.57104	0.00000
20 K	1 DZZ	0.00000	0.00000	0.00000	0.57104	0.00000
21 K	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 K	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

23 K	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		16	17	18	19	20
Eigenvalues:		-0.01763	-0.01763	0.05446	0.05446	0.05446
		A	A	A	A	A
1 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 K	1 PX	-0.02718	0.01283	0.00000	0.00000	0.00000
4 K	1 PY	0.06091	-0.00058	0.00000	0.00000	0.00000
5 K	1 PZ	0.00584	0.06572	0.00000	0.00000	0.00000
6 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 K	1 PX	0.10294	-0.04857	0.00000	0.00000	0.00000
8 K	1 PY	-0.23068	0.00218	0.00000	0.00000	0.00000
9 K	1 PZ	-0.02212	-0.24887	0.00000	0.00000	0.00000
10 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 K	1 PX	-0.65476	0.30896	0.00000	0.00000	0.00000
12 K	1 PY	1.46732	-0.01389	0.00000	0.00000	0.00000
13 K	1 PZ	0.14067	1.58299	0.00000	0.00000	0.00000
14 K	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
15 K	1 PX	0.61587	-0.29061	0.00000	0.00000	0.00000
16 K	1 PY	-1.38018	0.01307	0.00000	0.00000	0.00000
17 K	1 PZ	-0.13231	-1.48898	0.00000	0.00000	0.00000
18 K	1 DXX	0.00000	0.00000	-0.93848	-0.34532	0.00233
19 K	1 DYY	0.00000	0.00000	0.17018	0.98539	-0.00666
20 K	1 DZZ	0.00000	0.00000	0.76830	-0.64007	0.00433
21 K	1 DXY	0.00000	0.00000	0.00000	-0.00018	-0.01318
22 K	1 DXZ	0.00000	0.00000	0.00000	-0.00471	-0.71341
23 K	1 DYZ	0.00000	0.00000	0.00000	0.00485	0.70059

MO:		21	22	23
Eigenvalues:		0.05446	0.05446	0.17578
		A	A	A
1 K	1 S	0.00000	0.00000	0.00437
2 K	1 S	0.00000	0.00000	0.00928
3 K	1 PX	0.00000	0.00000	0.00000
4 K	1 PY	0.00000	0.00000	0.00000
5 K	1 PZ	0.00000	0.00000	0.00000
6 K	1 S	0.00000	0.00000	0.12771
7 K	1 PX	0.00000	0.00000	0.00000
8 K	1 PY	0.00000	0.00000	0.00000
9 K	1 PZ	0.00000	0.00000	0.00000
10 K	1 S	0.00000	0.00000	8.62620
11 K	1 PX	0.00000	0.00000	0.00000
12 K	1 PY	0.00000	0.00000	0.00000
13 K	1 PZ	0.00000	0.00000	0.00000
14 K	1 S	0.00000	0.00000	-2.58935
15 K	1 PX	0.00000	0.00000	0.00000
16 K	1 PY	0.00000	0.00000	0.00000
17 K	1 PZ	0.00000	0.00000	0.00000
18 K	1 DXX	0.00000	0.00006	-2.95772
19 K	1 DYY	0.00000	-0.00018	-2.95772
20 K	1 DZZ	0.00000	0.00012	-2.95772
21 K	1 DXY	0.86355	-0.50410	0.00000
22 K	1 DXZ	0.34511	0.60985	0.00000
23 K	1 DYZ	0.36768	0.61153	0.00000

** Archive file written to unit 12 **

```
  Total Cpu time:        0 mins.  2.31 secs.
  Total Wall time:       0 mins.  2.64 secs.

  Calculation finished: Fri Sep 18 13:41:25 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.07 secs.
```

```
SPARTAN AB INITIO PROGRAM: SGI/R4K        Release 5.0.1
  (Job run on hutton)



  Calculation started: Fri Sep 18 13:43:02 1998

  Run type: Single point energy
  Model: UHF/3-21G(*)
  Number of shells:   6
     1 S shells
     4 SP shells
     1 6D shells
  Number of basis functions:  23
  Number of electrons:  19
  Use of molecular symmetry disabled
  Molecular charge:   1
  Spin multiplicity:  2

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------

    Ca Ca1         -0.0000001     2.0502961    -2.0786987

  Point Group = C1  Order =  1 Nsymop =  1
  This system has   0 degrees of freedom

  UHF direct SCF procedure requested

  Energy converged to 0.28E-09 in  12 cycles  <S**2> = 0.7502

  E(HF)  =    -673.2308061 a.u.

  Alpha Spin Molecular Orbital Coefficients

  MO:                   1         2         3         4         5

  Eigenvalues:    -148.62398  -17.00369  -13.79276  -13.79276  -13.79276

                        A         A         A         A         A
   1 Ca  1 S        -0.98577   -0.30638    0.00000    0.00000    0.00000
   2 Ca  1 S        -0.05167    1.01375    0.00000    0.00000    0.00000
   3 Ca  1 PX        0.00000    0.00000    0.36508    0.86546   -0.30435
   4 Ca  1 PY        0.00000    0.00000   -0.83873    0.18215   -0.48814
   5 Ca  1 PZ        0.00000    0.00000   -0.37171    0.43902    0.80251
   6 Ca  1 S         0.01415    0.05518    0.00000    0.00000    0.00000
   7 Ca  1 PX        0.00000    0.00000    0.01471    0.03487   -0.01226
   8 Ca  1 PY        0.00000    0.00000   -0.03380    0.00734   -0.01967
   9 Ca  1 PZ        0.00000    0.00000   -0.01498    0.01769    0.03234
  10 Ca  1 S        -0.02954   -0.07607    0.00000    0.00000    0.00000
  11 Ca  1 PX        0.00000    0.00000   -0.00368   -0.00873    0.00307
  12 Ca  1 PY        0.00000    0.00000    0.00846   -0.00184    0.00492
  13 Ca  1 PZ        0.00000    0.00000    0.00375   -0.00443   -0.00809
  14 Ca  1 S         0.00027    0.00234    0.00000    0.00000    0.00000
  15 Ca  1 PX        0.00000    0.00000    0.00204    0.00484   -0.00170
  16 Ca  1 PY        0.00000    0.00000   -0.00469    0.00102   -0.00273
  17 Ca  1 PZ        0.00000    0.00000   -0.00208    0.00245    0.00448
  18 Ca  1 DXX       0.01188    0.02957    0.00000    0.00000    0.00000
  19 Ca  1 DYY       0.01188    0.02957    0.00000    0.00000    0.00000
```

20 Ca	1 DZZ	0.01188	0.02957	0.00000	0.00000	0.00000
21 Ca	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 Ca	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23 Ca	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		6	7	8	9	10
Eigenvalues:		-2.49327	-1.58201	-1.58201	-1.58201	-0.41543
		A	A	A	A	A
1 Ca	1 S	-0.10620	0.00000	0.00000	0.00000	-0.02863
2 Ca	1 S	0.40404	0.00000	0.00000	0.00000	0.11428
3 Ca	1 PX	0.00000	-0.27504	-0.12259	0.17850	0.00000
4 Ca	1 PY	0.00000	-0.20319	0.04637	-0.28125	0.00000
5 Ca	1 PZ	0.00000	0.07486	-0.32459	-0.10759	0.00000
6 Ca	1 S	-1.05597	0.00000	0.00000	0.00000	-0.32547
7 Ca	1 PX	0.00000	0.81352	0.36261	-0.52797	0.00000
8 Ca	1 PY	0.00000	0.60101	-0.13714	0.83189	0.00000
9 Ca	1 PZ	0.00000	-0.22141	0.96008	0.31824	0.00000
10 Ca	1 S	-0.00706	0.00000	0.00000	0.00000	1.11710
11 Ca	1 PX	0.00000	0.04459	0.01987	-0.02894	0.00000
12 Ca	1 PY	0.00000	0.03294	-0.00752	0.04559	0.00000
13 Ca	1 PZ	0.00000	-0.01213	0.05262	0.01744	0.00000
14 Ca	1 S	0.00877	0.00000	0.00000	0.00000	0.05669
15 Ca	1 PX	0.00000	-0.01814	-0.00809	0.01177	0.00000
16 Ca	1 PY	0.00000	-0.01340	0.00306	-0.01855	0.00000
17 Ca	1 PZ	0.00000	0.00494	-0.02141	-0.00710	0.00000
18 Ca	1 DXX	-0.00653	0.00000	0.00000	0.00000	-0.05737
19 Ca	1 DYY	-0.00653	0.00000	0.00000	0.00000	-0.05737
20 Ca	1 DZZ	-0.00653	0.00000	0.00000	0.00000	-0.05737
21 Ca	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 Ca	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23 Ca	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		11	12	13	14	15
Eigenvalues:		-0.14450	-0.14450	-0.14450	-0.04869	-0.01587
		A	A	A	A	A
1 Ca	1 S	0.00000	0.00000	0.00000	-0.00977	0.00000
2 Ca	1 S	0.00000	0.00000	0.00000	0.08925	0.00000
3 Ca	1 PX	0.05099	0.04718	0.01419	0.00000	0.06447
4 Ca	1 PY	0.02561	-0.00793	-0.06564	0.00000	0.03034
5 Ca	1 PZ	-0.04209	0.05233	-0.02274	0.00000	-0.00129
6 Ca	1 S	0.00000	0.00000	0.00000	0.05520	0.00000
7 Ca	1 PX	-0.18075	-0.16724	-0.05031	0.00000	-0.23595
8 Ca	1 PY	-0.09078	0.02811	0.23268	0.00000	-0.11104
9 Ca	1 PZ	0.14920	-0.18550	0.08062	0.00000	0.00471
10 Ca	1 S	0.00000	0.00000	0.00000	1.76964	0.00000
11 Ca	1 PX	0.50300	0.46542	0.14002	0.00000	1.36614
12 Ca	1 PY	0.25263	-0.07823	-0.64753	0.00000	0.64294
13 Ca	1 PZ	-0.41521	0.51623	-0.22436	0.00000	-0.02725
14 Ca	1 S	0.00000	0.00000	0.00000	-2.12677	0.00000
15 Ca	1 PX	0.27076	0.25053	0.07537	0.00000	-1.42594
16 Ca	1 PY	0.13599	-0.04211	-0.34856	0.00000	-0.67108
17 Ca	1 PZ	-0.22351	0.27788	-0.12077	0.00000	0.02844
18 Ca	1 DXX	0.00000	0.00000	0.00000	0.04931	0.00000
19 Ca	1 DYY	0.00000	0.00000	0.00000	0.04931	0.00000
20 Ca	1 DZZ	0.00000	0.00000	0.00000	0.04931	0.00000
21 Ca	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 Ca	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

23 Ca	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		16	17	18	19	20
Eigenvalues:		-0.01587	-0.01587	0.00086	0.00086	0.00086
		A	A	A	A	A
1 Ca	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 Ca	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 Ca	1 PX	0.00688	0.02958	0.00000	0.00000	0.00000
4 Ca	1 PY	-0.01754	-0.06206	0.00000	0.00000	0.00000
5 Ca	1 PZ	-0.06873	0.01880	0.00000	0.00000	0.00000
6 Ca	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 Ca	1 PX	-0.02519	-0.10825	0.00000	0.00000	0.00000
8 Ca	1 PY	0.06419	0.22709	0.00000	0.00000	0.00000
9 Ca	1 PZ	0.25153	-0.06880	0.00000	0.00000	0.00000
10 Ca	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 Ca	1 PX	0.14588	0.62676	0.00000	0.00000	0.00000
12 Ca	1 PY	-0.37169	-1.31489	0.00000	0.00000	0.00000
13 Ca	1 PZ	-1.45637	0.39836	0.00000	0.00000	0.00000
14 Ca	1 S	0.00000	0.00000	0.00000	0.00000	0.00000
15 Ca	1 PX	-0.15226	-0.65420	0.00000	0.00000	0.00000
16 Ca	1 PY	0.38796	1.37244	0.00000	0.00000	0.00000
17 Ca	1 PZ	1.52012	-0.41580	0.00000	0.00000	0.00000
18 Ca	1 DXX	0.00000	0.00000	0.00012	-0.01298	-0.04120
19 Ca	1 DYY	0.00000	0.00000	-0.00081	0.01568	0.04838
20 Ca	1 DZZ	0.00000	0.00000	0.00069	-0.00270	-0.00718
21 Ca	1 DXY	0.00000	0.00000	0.61317	-0.71265	-0.33948
22 Ca	1 DXZ	0.00000	0.00000	-0.17864	0.29483	-0.93767
23 Ca	1 DYZ	0.00000	0.00000	0.76949	0.63633	0.05287

MO:		21	22	23
Eigenvalues:		0.00086	0.00086	0.44082
		A	A	A
1 Ca	1 S	0.00000	0.00000	-0.05026
2 Ca	1 S	0.00000	0.00000	0.20832
3 Ca	1 PX	0.00000	0.00000	0.00000
4 Ca	1 PY	0.00000	0.00000	0.00000
5 Ca	1 PZ	0.00000	0.00000	0.00000
6 Ca	1 S	0.00000	0.00000	-0.60320
7 Ca	1 PX	0.00000	0.00000	0.00000
8 Ca	1 PY	0.00000	0.00000	0.00000
9 Ca	1 PZ	0.00000	0.00000	0.00000
10 Ca	1 S	0.00000	0.00000	5.04702
11 Ca	1 PX	0.00000	0.00000	0.00000
12 Ca	1 PY	0.00000	0.00000	0.00000
13 Ca	1 PZ	0.00000	0.00000	0.00000
14 Ca	1 S	0.00000	0.00000	0.42344
15 Ca	1 PX	0.00000	0.00000	0.00000
16 Ca	1 PY	0.00000	0.00000	0.00000
17 Ca	1 PZ	0.00000	0.00000	0.00000
18 Ca	1 DXX	0.78962	-0.61208	-2.42113
19 Ca	1 DYY	-0.92407	-0.37881	-2.42113
20 Ca	1 DZZ	0.13446	0.99089	-2.42113
21 Ca	1 DXY	-0.03010	-0.00074	0.00000
22 Ca	1 DXZ	-0.04398	0.00010	0.00000
23 Ca	1 DYZ	0.01296	-0.00017	0.00000

Beta Spin Molecular Orbital Coefficients

MO:			1	2	3	4	5
Eigenvalues:			-148.62160	-16.99958	-13.79125	-13.79125	-13.79125
			A	A	A	A	A
1	Ca	1 S	-0.98577	-0.30637	0.00000	0.00000	0.00000
2	Ca	1 S	-0.05168	1.01368	0.00000	0.00000	0.00000
3	Ca	1 PX	0.00000	0.00000	0.36627	0.85883	-0.32126
4	Ca	1 PY	0.00000	0.00000	-0.83881	0.17407	-0.49098
5	Ca	1 PZ	0.00000	0.00000	-0.37041	0.45504	0.79416
6	Ca	1 S	0.01415	0.05536	0.00000	0.00000	0.00000
7	Ca	1 PX	0.00000	0.00000	0.01475	0.03458	-0.01293
8	Ca	1 PY	0.00000	0.00000	-0.03377	0.00701	-0.01977
9	Ca	1 PZ	0.00000	0.00000	-0.01491	0.01832	0.03197
10	Ca	1 S	-0.02955	-0.07639	0.00000	0.00000	0.00000
11	Ca	1 PX	0.00000	0.00000	-0.00367	-0.00862	0.00322
12	Ca	1 PY	0.00000	0.00000	0.00842	-0.00175	0.00493
13	Ca	1 PZ	0.00000	0.00000	0.00372	-0.00457	-0.00797
14	Ca	1 S	0.00027	0.00234	0.00000	0.00000	0.00000
15	Ca	1 PX	0.00000	0.00000	0.00204	0.00478	-0.00179
16	Ca	1 PY	0.00000	0.00000	-0.00467	0.00097	-0.00273
17	Ca	1 PZ	0.00000	0.00000	-0.00206	0.00253	0.00442
18	Ca	1 DXX	0.01188	0.02970	0.00000	0.00000	0.00000
19	Ca	1 DYY	0.01188	0.02970	0.00000	0.00000	0.00000
20	Ca	1 DZZ	0.01188	0.02970	0.00000	0.00000	0.00000
21	Ca	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22	Ca	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23	Ca	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:			6	7	8	9	10
Eigenvalues:			-2.48169	-1.57722	-1.57722	-1.57722	-0.18254
			A	A	A	A	A
1	Ca	1 S	-0.10604	0.00000	0.00000	0.00000	0.02437
2	Ca	1 S	0.40331	0.00000	0.00000	0.00000	-0.08621
3	Ca	1 PX	0.00000	0.23278	-0.23077	0.12470	0.00000
4	Ca	1 PY	0.00000	0.18061	0.02010	-0.29995	0.00000
5	Ca	1 PZ	0.00000	-0.19023	-0.26331	-0.13219	0.00000
6	Ca	1 S	-1.05377	0.00000	0.00000	0.00000	0.31128
7	Ca	1 PX	0.00000	-0.68884	0.68289	-0.36900	0.00000
8	Ca	1 PY	0.00000	-0.53445	-0.05949	0.88760	0.00000
9	Ca	1 PZ	0.00000	0.56291	0.77918	0.39117	0.00000
10	Ca	1 S	-0.02430	0.00000	0.00000	0.00000	-0.54393
11	Ca	1 PX	0.00000	-0.03142	0.03115	-0.01683	0.00000
12	Ca	1 PY	0.00000	-0.02438	-0.00271	0.04049	0.00000
13	Ca	1 PZ	0.00000	0.02568	0.03554	0.01784	0.00000
14	Ca	1 S	0.00952	0.00000	0.00000	0.00000	-0.49715
15	Ca	1 PX	0.00000	0.01322	-0.01311	0.00708	0.00000
16	Ca	1 PY	0.00000	0.01026	0.00114	-0.01704	0.00000
17	Ca	1 PZ	0.00000	-0.01081	-0.01496	-0.00751	0.00000
18	Ca	1 DXX	-0.00004	0.00000	0.00000	0.00000	-0.01366
19	Ca	1 DYY	-0.00004	0.00000	0.00000	0.00000	-0.01366
20	Ca	1 DZZ	-0.00004	0.00000	0.00000	0.00000	-0.01366
21	Ca	1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22	Ca	1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23	Ca	1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	11	12	13	14	15

Eigenvalues:	-0.10898	-0.10898	-0.10898	-0.03066	0.00158
	A	A	A	A	A
1 Ca 1 S	0.00000	0.00000	0.00000	-0.01403	0.00000
2 Ca 1 S	0.00000	0.00000	0.00000	0.10475	0.00000
3 Ca 1 PX	-0.02741	0.02661	0.03837	0.00000	-0.04428
4 Ca 1 PY	-0.03463	0.01825	-0.03740	0.00000	-0.06273
5 Ca 1 PZ	0.03131	0.04348	-0.00778	0.00000	0.02843
6 Ca 1 S	0.00000	0.00000	0.00000	0.00428	0.00000
7 Ca 1 PX	0.09697	-0.09411	-0.13571	0.00000	0.16185
8 Ca 1 PY	0.12252	-0.06454	0.13230	0.00000	0.22930
9 Ca 1 PZ	-0.11075	-0.15381	0.02753	0.00000	-0.10391
10 Ca 1 S	0.00000	0.00000	0.00000	1.78968	0.00000
11 Ca 1 PX	-0.20187	0.19592	0.28252	0.00000	-0.87396
12 Ca 1 PY	-0.25505	0.13436	-0.27541	0.00000	-1.23817
13 Ca 1 PZ	0.23055	0.32018	-0.05730	0.00000	0.56111
14 Ca 1 S	0.00000	0.00000	0.00000	-2.07924	0.00000
15 Ca 1 PX	-0.33938	0.32938	0.47497	0.00000	0.79794
16 Ca 1 PY	-0.42878	0.22588	-0.46302	0.00000	1.13046
17 Ca 1 PZ	0.38759	0.53829	-0.09634	0.00000	-0.51229
18 Ca 1 DXX	0.00000	0.00000	0.00000	0.12048	0.00000
19 Ca 1 DYY	0.00000	0.00000	0.00000	0.12048	0.00000
20 Ca 1 DZZ	0.00000	0.00000	0.00000	0.12048	0.00000
21 Ca 1 DXY	0.00000	0.00000	0.00000	0.00000	0.00000
22 Ca 1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
23 Ca 1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	16	17	18	19	20
Eigenvalues:	0.00158	0.00158	0.02655	0.02655	0.02655
	A	A	A	A	A
1 Ca 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
2 Ca 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
3 Ca 1 PX	-0.03229	0.06084	0.00000	0.00000	0.00000
4 Ca 1 PY	-0.01095	-0.05147	0.00000	0.00000	0.00000
5 Ca 1 PZ	-0.07444	-0.01882	0.00000	0.00000	0.00000
6 Ca 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
7 Ca 1 PX	0.11801	-0.22238	0.00000	0.00000	0.00000
8 Ca 1 PY	0.04002	0.18813	0.00000	0.00000	0.00000
9 Ca 1 PZ	0.27211	0.06878	0.00000	0.00000	0.00000
10 Ca 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
11 Ca 1 PX	-0.63723	1.20076	0.00000	0.00000	0.00000
12 Ca 1 PY	-0.21607	-1.01586	0.00000	0.00000	0.00000
13 Ca 1 PZ	-1.46934	-0.37137	0.00000	0.00000	0.00000
14 Ca 1 S	0.00000	0.00000	0.00000	0.00000	0.00000
15 Ca 1 PX	0.58180	-1.09631	0.00000	0.00000	0.00000
16 Ca 1 PY	0.19728	0.92749	0.00000	0.00000	0.00000
17 Ca 1 PZ	1.34152	0.33906	0.00000	0.00000	0.00000
18 Ca 1 DXX	0.00000	0.00000	0.00199	-0.00037	0.00085
19 Ca 1 DYY	0.00000	0.00000	0.00003	0.00042	0.29638
20 Ca 1 DZZ	0.00000	0.00000	-0.00202	-0.00005	-0.29723
21 Ca 1 DXY	0.00000	0.00000	0.32421	0.78119	-0.50140
22 Ca 1 DXZ	0.00000	0.00000	-0.80302	0.52538	0.26455
23 Ca 1 DYZ	0.00000	0.00000	0.50005	0.33721	0.74910

MO:	21	22	23
Eigenvalues:	0.02655	0.02655	0.46518
	A	A	A

```
  1 Ca  1 S         0.00000    0.00000   -0.05192
  2 Ca  1 S         0.00000    0.00000    0.21622
  3 Ca  1 PX        0.00000    0.00000    0.00000
  4 Ca  1 PY        0.00000    0.00000    0.00000
  5 Ca  1 PZ        0.00000    0.00000    0.00000
  6 Ca  1 S         0.00000    0.00000   -0.61688
  7 Ca  1 PX        0.00000    0.00000    0.00000
  8 Ca  1 PY        0.00000    0.00000    0.00000
  9 Ca  1 PZ        0.00000    0.00000    0.00000
 10 Ca  1 S         0.00000    0.00000    5.13348
 11 Ca  1 PX        0.00000    0.00000    0.00000
 12 Ca  1 PY        0.00000    0.00000    0.00000
 13 Ca  1 PZ        0.00000    0.00000    0.00000
 14 Ca  1 S         0.00000    0.00000    0.36773
 15 Ca  1 PX        0.00000    0.00000    0.00000
 16 Ca  1 PY        0.00000    0.00000    0.00000
 17 Ca  1 PZ        0.00000    0.00000    0.00000
 18 Ca  1 DXX      -0.00296    0.99999   -2.41928
 19 Ca  1 DYY      -0.81209   -0.50266   -2.41928
 20 Ca  1 DZZ       0.81505   -0.49733   -2.41928
 21 Ca  1 DXY      -0.18228   -0.00047    0.00000
 22 Ca  1 DXZ       0.09565    0.00185    0.00000
 23 Ca  1 DYZ       0.27402   -0.00069    0.00000

   ** Archive file written to unit 12 **

  Total Cpu time:        0 mins.  4.03 secs.
  Total Wall time:       0 mins.  4.57 secs.

  Calculation finished: Fri Sep 18 13:43:07 1998

SPARTAN PROPERTIES PACKAGE: SGI/R4K        Release 5.0.1
Atom 1 is unattached
Unable to type atom 1 for Ghose/Crippen analysis

  Total Cpu time:   0 mins.  0.08 secs.
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