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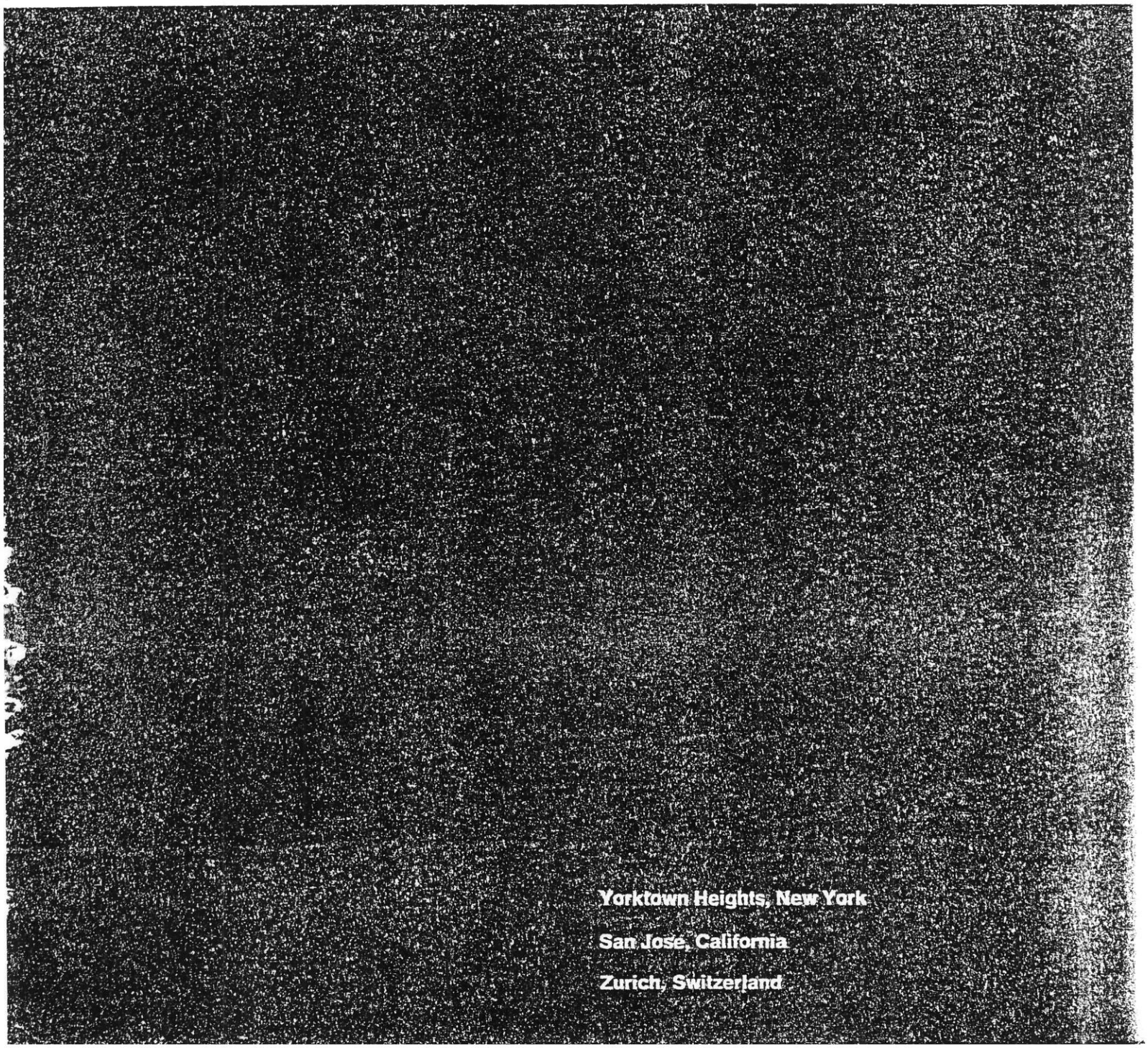

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GAUSSIAN BASIS SETS FOR THE ATOMS H - Ne

FOR USE IN MOLECULAR CALCULATIONS

F. B. van Duijneveldt[†]

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ABSTRACT: This report contains a collection of atomic SCF functions for the atoms H through Ne employing optimized basis sets of Gaussian-type orbitals (GTO). A wide range of basis set sizes has been covered, including 13 s sets for Li and Be, and 13s8p sets for B-F, thus bringing near-Hartree-Fock calculations on molecules containing these atoms within reach. New 6s3p sets containing two s-GTO's in the 2s valence region are reported as well. An introductory section provides an explanation of the tables and some notes on molecular applications using these sets.

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1. INTRODUCTION

This report contains atomic basis sets of Gaussian-type orbitals (GTO) for use in molecular calculations. Of the various types of GTO basis sets that one encounters in the literature, only a single type has been considered in this volume: within each basis set a single, uncontracted GTO set is used for all atomic SCF orbitals of a given symmetry,[1] and all GTO exponents have been determined by minimizing the Roothaan-Hartree-Fock atomic energy.[2] Although such basis sets have been available for several years,[3] especially through Huzinaga's early work, it was felt that their present widespread use has created a need for a collection of rigorously optimized sets of this kind, including some larger sets than were available so far.

The present volume contains such a collection for the atoms H through Ne.[4] Among the smaller sets that have been included, special mention should be made of some new 6s3p or (6/3) sets containing <u>two</u> s-GTO's in the 2s valence region. These sets are suitable candidates for use in molecular calculations at the single-ζ STO level. A wide choice of medium-size sets has been included for use in problems where higher accuracy is needed. Finally, the largest sets included (e.g., 13s8p for B up to F) are designed for calculations at the Hartree-Fock level.

The following introductory pages describe how the exponent optimization was carried out and they discuss the occurrence of multiple minima during this optimization. Next, the way in which the optimal basis sets are presented is described in some detail. Finally, we have included some notes on molecular applications and some Tables summarizing total energies obtained in the present work, as well as the corresponding Hartree-Fock values.

2. COMPUTATIONAL DETAILS

All calculations were carried out using the ATOMSCF program by Roos et al.[5] which is based on the atomic SCF program originally published by Roothaan and Bagus.[6] The program allows for automatic optimization of some or all orbital exponents (α_i) in the following way. The first step consists of one-dimensional optimizations for each of the exponents separately, using exponent increments given as input. This step is repeated once or twice and the exponent changes in the last two cycles are then employed in a simultaneous variation of all exponents until a minimum is reached. This allows for scaling and deformation of the exponent set. The whole procedure (steps 1 + 2) is repeated as often as desired. In most cases the optimization was carried on until the energy had become stable to about 1 part in 10^7, and 5 to 10 complete cycles were usually sufficient to attain this limit. The resulting exponents are thought to be optimal to within 1% in most cases.

The optimization of a large basis set by the above procedure is very time consuming. For example, one complete cycle (steps 1 + 2) for a 13/8 set took about 10 min. on the IBM 360/91. Starting exponents and exponent increments therefore had to be selected very carefully in order to assure convergence in as few cycles as possible. Initially, starting exponents were taken from the papers by Huzinaga and by Whitman and Hornback,[3] but in later work, and especially for large sets, they were obtained graphically from graphs as shown in Figure 1 for the nitrogen atom. The exponent increments employed varied from 0.01 α_i, to 0.05 α_i, depending on the absolute value of α_i.

Incidentally, Figure 1 shows that the α_i of a particular set are nearly equidistant on a logarithmic scale. This means that the ratio between successive exponents and hence the overlap integral between successive GTO's is nearly constant, thus avoiding dependency.[7]

3. MULTIPLE MINIMA

From Figure 1 it is clear that for small s-sets the space of the nitrogen s-exponents consists of two distinct regions, viz. a high-exponent region corresponding to the 1s AO and a low-exponent region corresponding to the outer lobe of the 2s AO. Starting from a (minimal) 2s set a third exponent has to go to the 1s region, since this contributes most to the energy; but in going from 5s to 6s, the energy improvements for adding the sixth exponent in the 1s or 2s region are about equal and two optimal solutions can now be obtained. Similar remarks hold for the 6s sets of all other atoms in the series Li-Ne, the main change being in the energetic importance of the 2s region. Thus for C up to Ne the '4-2' solution (having 2 GTO's in the 2s region) is the one of lowest energy, whereas for Li, Be and B the '5-1' solution has the lower energy (see Table 1).

In most molecular applications the '4-2' solution is the best to use, since it has more GTO's in the valence region. For this reason only the 4-2 solutions have been reported here, except for Li where (by error) a 5-1 set is given instead. For the reader's convenience a 4-2 solution for Li is presented in Table 2. Nearly optimal 5-1 sets for Li up to Ne may be found in refs. 3c and 4a.

Multiple minima may in principle occur for larger s-sets than 6s, and in a number of cases this resulted in slow convergence of the optimization

procedure. However, the Li 11s-set was the only other case where two optimal solutions could actually be obtained. The 9-2 solution presented here is the one of lowest energy, but in molecular work the 8-3 solution reported by Huzinaga[3b] is to be preferred.

4. EXPLANATION OF TABLES

Some 150 basis sets that resulted from the present work have been collected on pp. 1-77. Direct use was made of the machine output in order to reduce the risk of typographical errors. As an example, let us consider the boron atom (p. 17-26). Page 17 starts with some constants that are given only once for each atom, viz. the nuclear charge (5.0) and the vector coupling constants[6] characterizing the electronic state ($1s^2 2s^2 2p^1$, ^2P). Page 17 continues with the two smallest GTO sets that have been computed, viz. a 4/2 and a 5/2 set. Here 4/2 (or 4s2p) indicates that the basis set contains 4 s-type GTO's and 2 p-type GTO's in the x,y and z direction each. The s-type GTO's are normalized 1s Gaussians,

$$G1s(\alpha) = (2\alpha/\pi)^{3/4} \exp(-\alpha r^2),$$

differing in their orbital exponent (α) only. Likewise, the p-type GTO's are 2p-Gaussian given by

$$G2p(\alpha) = (128\alpha^5/\pi^3)^{1/4} x_j \exp(-\alpha r^2),$$

where x_j = x,y or z, as appropriate.

For atoms with occupied s and p AO's (such as boron) the title of each set (e.g., 'boron 4/2 derived source set') contains information on the extent of exponent optimization employed. In particular,

SOURCE indicates that all s and p exponents were optimized. This applies to 5/2 7/3 8/4 9/5 11/6 12/7 13/8 and 14/9 sets.

DERIVED SOURCE indicates that all k s-exponents were optimized, but the 1 p-exponents were copied from the (k + 1)/1 set. The 4/2 6/3 and 10/6 sets are of this type.

DERIVED indicates that all exponents were copied from the appropriate 'source' or 'derived source' sets. For example, the s-exponents of 6/2 are taken from 6/3 and the p-exponents from 5/2. There is no point in re-optimizing a derived set since the energy gain would usually be less than 0.00002 a.u. (This is due to s,p separability, as first noted by Whitman and Hornback.[3c])

Apart from the title, the listing of a basis set (e.g., of the 4/2 set) consists of the following:

(1) The total Hartree-Fock energy, obtained in the final SCF calculation (-24.33612 a.u.).

(2) The potential (V) and kinetic (T) components of the total HF energy, also in atomic units.

(3) The ratio V/T which according to the virial theorem should equal -2 for a perfectly scaled (but not necessarily optimal) basis set (the value here is -1.99995).

(4) The exponents α_i for the s-type and p-type GTO's (as obtained from the exponent optimization procedure or as copied from a different set) that were used in the final SCF calculation. As noted before, the quantum numbers of the s- and p-type GTO's are always 1 and 2, respectively. Note that the same exponents α_i are used in the expansion of 2p-AO's of

different symmetry (x,y or z), and hence only a single set of p-exponents is listed.

(5) The orbital energies of the 1s, 2s and 2p AO's, in this order, as obtained in the final SCF calculation. (ε_{1s} = -7.63187, ε_{2s} = -0.47787, ε_{2p} = -0.27449, all in a.u.)

(6) The expansion coefficients of the various GTO's in the 1s, 2s and 2p AO's (ϕ), obtained as the eigenvectors of the final HF matrix. Thus

$$\begin{aligned}\phi_{1s} &= 0.032968\ \text{G1s}(0.189977)\\ &+ 0.663270\ \text{G1s}(3.37977)\\ &+ 0.387633\ \text{G1s}(16.0070)\\ &+ 0.069252\ \text{G1s}(106.949).\end{aligned}$$

The same four 1s-Gaussians are employed in the expansion of ϕ_{2s}:

$$\begin{aligned}\phi_{2s} &= 1.034928\ \text{G1s}(0.189977)\\ &- 0.212940\ \text{G1s}(3.37977)\\ &- 0.087386\ \text{G1s}(16.0070)\\ &- 0.013701\ \text{G1s}(106.949),\end{aligned}$$

whereas ϕ_{2p} is given by

$$\begin{aligned}\phi_{2p} &= 0.809935\ \text{G2p}(0.168230)\\ &+ 0.328902\ \text{G2p}(0.924520).\end{aligned}$$

Note that the same radial functions are employed for ϕ_{2px} ϕ_{2py} and ϕ_{2pz}, and hence only a single set of p-coefficients is listed.

5. NOTES ON MOLECULAR APPLICATIONS

The availability of adequate atomic basis sets is merely a first step in performing molecular SCF computations. Those who wish to employ basis

sets such as in the present volume will have to choose their basis set size, contraction scheme, and polarization functions, to mention a few. The following remarks are intended to provide some additional information on these matters.

(1) Balanced Sets

The problem here is to find the right balance between the number of s- and p-GTO's on an atom having occupied s and p shells, and to decide how many s-GTO's one should use on a 'light' atom (H,He) in conjunction with s/p sets of a given size on larger atoms. In order to determine a reasonable s/p ratio, one might compare the absolute and relative energy improvements resulting from adding s or p functions to a basis of given size. A little consideration then shows that the s/p ratio of the following sets is too low:

2/1 3/2 4/3 6/4 8/5 9/6 10/7 12/8 , (A)

whereas that of the following is too high ,

4/1 5/2 7/3 9/4 11/5 12/6 13/7 15?/8 . (B)

These results are for N, but very similar results are obtained for all atoms B-Ne. A further argument that one might consider in choosing the s/p ratio is that the valence AO's should be described equally well and so the relative errors in ε_{2s} and ε_{2p} should be roughly equal. This yields s/p ratio's near those of A. On the other hand, since adding a p to nsmp means adding <u>three</u> functions it is far cheaper, computationally, to adopt s/p ratio's near those of B.

Next, the number of s-GTO's in H or He to be used together with an s/p set of given size may be determined by requiring that the relative accuracy (relative to the HF-limit) of the atomic energies involved be about equal. For nsmp sets intermediate between A and B this implies the use of m or (m + 1) s-GTO's on H or He. In practice it turns out[8] that very little is lost by using only m s-GTO's.

It should be noted that the relative accuracy of an nsmp set decreases in the series B-Ne, to the extent that a Ne set has to be about 1s1p larger than a B set if the same relative accuracy is to be attained. In large-basis calculations this can probably be ignored, but in small-basis calculations on hetero-atomic molecules this causes severe problems since wrong polarities can easily result unless the absolute errors in the valence-AO's are about equal.[9]

(2) Basis Set Size

The sets presented here span a wide range of accuracies. For work at the level of minimal-basis STO calculations a (6,3/3) set will usually be adequate (i.e., a 6s or 6s3p set on the 'heavy' atom and a 3s set on H or He). The 'heavy' atom 6s sets have the special advantage that they are the smallest sets having 2 GTO's in the 2s valence region, and hence only four GTO's are spent on describing the core region. For discussions of what can be done at this level of accuracy see the work by Pople and co-workers.[10] Calculation at the double-zeta STO level require something like (9,5/5) sets. When augmented by suitable polarization functions (see below), such a set will be adequate for most applications of interest to chemists. The (11,6/6) and (12,7/7) sets are roughly at triple-zeta STO level. They give atomic energies within some 0.001 a.u. from the HF-limit. Finally, (13,8/8)

calculations on molecules practically represent the isotropic limit, i.e., no further improvement can be obtained by adding more functions of the same type. It should be noted that in small-basis calculations one needs about 3 GTO per STO, but this decreases to about 2 GTO per STO in large-basis calculations, which implies that the advantage of using GTO's rather than STO's increases with the size of the basis.

(3) Contraction

In order to reduce the number of integrals that must be stored and handled in setting up the HF-matrix, and in order to reduce the size of this matrix, it is useful to contract the primitive basis of GTO's to some extent. Molecular calculations show[8,11] that contraction of the innermost s- and p-GTO's can be carried through without any loss in accuracy. However, in contracting GTO's in the valence region one should be very careful. In many cases the gain in flexibility by not contracting the outer GTO's more than offsets the increase in computation time (which for an efficient program should be small anyway). An additional advantage of loosely contracted basis sets is that free-atom exponents need no scaling when used in a molecular environment.[8]

(4) Polarization Functions

These should be added to the isotropic sets described above if one is to obtain bond lengths, bond angles, dipole moments and other properties in agreement with the Hartree-Fock values and, more important, with experiment. For example, flexible isotropic calculations (e.g., using a (11,6/6) basis) yield a planar geometry for NH_3,[12] but a single set of polarization functions (p_x,p_y,p_z on H, and six cartesian d-functions

on N, to give a (11,6,1/6,1) basis) is sufficient to produce a correct geometry.[8,12] Orbital exponents for these functions can be inferred from the corresponding STO exponents reported in the literature,[13] or they can be found by direct optimization in a molecular environment. Average exponents taken from extensive optimization work on CH_4 and HF are listed below.

Orbital Exponents for Polarization Functions (GTO)

using 1 set:	$\alpha_p(H) = 1.0$	$\alpha_d(C \text{ or } F) = 1.0$
using 2 sets:	$\alpha_p(H) = 0.25/1.4$	$\alpha_d(C \text{ or } F) = 0.35/1.5$

As the optimal exponents in the two molecules were very similar, these values can probably safely be used in other molecules containing C, N, O, F and H, especially since it does not make much difference if the exponents are not rigorously optimal. For CH_4 and HF the energy improvement from adding one set of polarization functions was about 0.02 a.u. while a second set gave about 0.002 a.u. This means that for such molecules a (11,6/6) set - which gives an energy within 0.004 a.u. from the isotropic limit - is a waste of accuracy, unless at least a single set (p_H, d_x) is included as well. In practice, even smaller sets such as (9,5/5) can usefully be augmented by such functions. In (2) we noted the favorable performance of GTO's with respect to STO's in large basis calculations. This trend becomes even more pronounced when polarization functions are added to the basis, for here a single GTO is nearly as effective as a single STO. GTO's therefore form an efficient basis for obtaining near Hartree-Fock results, except for properties such as the electron density at a nucleus where STO's remain superior.

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FOOTNOTES AND REFERENCES

1. Basis sets built from optimized contracted Gaussians may be found in the following papers. J. L. Whitten, J. Chem. Phys. 44, 359 (1966); S. Huzinaga and C. Arnau, ibid. 52, 2224 (1970); R. Ditchfield, W. J. Hehre and J. A. Pople, ibid. 54, 724 (1971) and refs. therein.

2. Basis sets obtained by least-squares fitting to STO's and HF-AO's are described by R. F. Stewart, J. Chem. Phys. 52, 431 (1970) and references therein.

3. (a) S. Huzinaga, J. Chem. Phys. 42, 1293 (1965). See also (b) S. Huzinaga and Y. Sakai, ibid. 50, 1371 (1969); (c) D. R. Whitman and C. J. Hornback, ibid. 51, 398 (1969); (d) B. Roos and P. Siegbahn, Theor. chim. Acta 17, 209 (1970).

4. (a) Basis sets for heavier atoms may be found in Huzinaga's recent compilation, S. Huzinaga, D. McWilliams and B. Domsky, J. Chem. Phys. 54, 2283 (1971). See also (b) A. Veillard, Theor. chim. Acta 12, 405 (1968); H. Basch, C. J. Hornback and J. W. Moskowitz, J. Chem. Phys. 51, 1311 (1969); A. J. H. Wachters, ibid. 52, 1033 (1970); R. F. Stewart and W. J. Hehre, ibid. 52, 5243 (1970); T. A. Claxton and N. A. Smith, Theor. chim. Acta 22, 378 (1971) as well as refs. 3b and 3d.

5. B. Roos, C. Salez, A. Veillard and E. Clementi, A General Program for Calculation of Atomic SCF Orbitals by the Expansion Method, IBM Technical Report RJ 518, August 12, 1968.

6. C. C. J. Roothaan and P. S. Bagus, Methods in Computational Physics, vol. II, Academic Press, New York, 1963, p. 47.

7. C. M. Reeves, J. Chem. Phys. 39, 1 (1963).

8. Calculations in a number of different bases, mainly on HF (F. B. van Duijneveldt, to be published).

9. H. B. Jansen, Ph.D. Thesis, Vrije Universiteit, Amsterdam (to be submitted).

10. J. A. Pople, Acc. Chem. Res. 217 (1970).

11. T. H. Dunning, J. Chem. Phys. 53, 2823 (1970).

12. A. Rauk, L. C. Allen and E. Clementi, J. Chem. Phys. 52, 4133 (1970).

13. For example, one might use $\alpha = \zeta^2/2n$ where α and ζ are the GTO and STO orbital exponents, respectively, and n is the main quantum number. The maximum in the radial distribution function of these orbitals will then occur at the same distance.

14. E. Clementi, Tables of Atomic Functions, Supplement to IBM J. Res. and Develop. 9, 2 (1965).

Table 1. Optimal energies (a.u.) for 6s3p sets having one or two GTO's in the 2s region

	Li	B	N	F	
'5-1'	-7.428	-24.492	-54.283	-99.129	from ref. 4a
'4-2'	-7.420[a]	-24.491	-54.295	-99.161	present work

a) From Table 2.

Table 2. Non-optimal 6s set for Li (^{2}S)[a]

α_1	C_{1s}	C_{2s}
101.390	0.020829	-0.003281
15.3116	0.138816	-0.023501
3.40235	0.447529	-0.077006
0.87357	0.528307	-0.182094
0.08000	0.044654	0.403662
0.03300	-0.020433	0.665602

ε_{1s} = -2.47042 ε_{2s} = -0.19590

total energy = -7.42023 virial theorem = -2.0006

a) Partly optimized by H.B. Jansen (Vrije Universiteit, Amsterdam) whose cooperation is gratefully acknowledged.

Table 3. Summary of Hartree-Fock results for N-He (in a.u.)

atom	state	total energy	ε_{1s}	ε_{2s}	ε_{2p}	ref
He	^1S	-2.861680	-0.91796			a
Li	^2S	-7.432727	-2.477741	-0.196323		b
Be	^1S	-14.573022	-4.732667	-0.309269		c
B	^2P	-24.529059	-7.695334	-0.494706	-0.309856	b
C	^3P	-37.688619	-11.325519	-0.705627	-0.433340	b
N	^4S	-54.400924	-15.629054	-0.945323	-0.567589	b
O	^3P	-74.809398	-20.668658	-1.244315	-0.631906	b
F	^2P	-99.409354	-26.382762	-1.572535	-0.730018	b
Ne	^1S	-128.54708	-32.77238	-1.93039	-0.85037	c

a) Analytical results from ref. 14.

b) Numerical results by P. S. Bagus (unpublished).

c) Analytical results from ref. 4a.

Table 4. Total energies (a.u.) of ns GTO sets for H,Ne,Li and Be (from pp. 1-16)

basis	$H(^2S)$	$He(^1S)$	$Li(^2S)$	$Be(^1S)$
1s	-0.424413[a]	-2.300987[a]	-	-
2s	-0.485813	-2.747066	-	-12.25020
3s	-0.496979	-2.835680	-	-14.12005
4s	-0.499278	-2.855160	-7.376906	-14.46790
5s	-0.499810	-2.859895	-7.418181	-14.53986
6s	-0.499946	-2.861153	-7.427859	-14.55159[b]
7s	-0.499983[3]	-2.861514	-7.429359	-14.56724
8s	-0.499994[5]	-2.861625	-7.431751	-14.57124
9s	-0.499998[1]	-2.861661	-7.432413	-14.57233
10s	-0.499999[2]	-2.861673	-7.432572	-14.57258
11s	-	-	-7.432643	-14.57287
12s	-	-	-7.432690	-14.57295
13s	-	-	-7.432710	-14.57299

a) From ref. 3a.

b) For 6s set with 2 GTO in valence region. An energy of -14.55638 is obtained for the alternative set with 1 GTO in the valence region.

Table 5. Total energies (a.u.) of nsmp GTO sets for B-Ne (from pp. 17-77).

basis[a]	B(^{2}P)	C(^{3}P)	N(^{4}S)	O(^{3}P)	F(^{2}P)	Ne(^{1}S)
4s 2p S	-24.33612	-37.35574	-53.86289	-73.97518	-98.18176	-126.81594
5s 2p SP	-24.44726	-37.51525	-54.07992	-74.25847	-98.54046	-127.25920
6s 2p	-24.47177	-	-54.14217	-74.34638	-98.65808	-127.41052
5s 3p	-24.46617	-37.58116	-54.23128	-74.55292	-99.04109	-128.03932
6s 3p S	-24.49078	-37.62297	-54.29461	-74.64241	-99.16103	-128.19400
7s 4p	-24.52051	-37.66512	-54.35148	-74.71622	-99.25406	-128.30852
7s 4p	-24.51881	-37.67132	-54.37337	-74.76656	-99.34620	-128.45801
8s 4p SP	-24.52487	-37.67994	-54.38504	-74.78174	-99.36540	-128.48170
9s 4p	-24.52649	-37.68224	-54.38837	-74.78615	-99.37104	-128.48873
9s 5p SP	-24.52747	-37.68555	-54.39583	-74.80095	-99.39635	-128.52822
10s 5p	-24.52808	-37.68665	-54.39729	-74.80304	-99.39905	-128.53180
10s 6p S	-24.52831	-37.68742	-54.39904	-74.80654	-99.40509	-128.54122
11s 6p SP	-24.52873	-37.68802	-54.39990	-74.80762	-99.40653	-128.54288
12s 6p	-24.52887	-37.68820	-54.40016	-74.80796	-99.40694	-128.54340
11s 7p	-24.52879	-37.68820	-54.40033	-74.80849	-99.40804	-128.54522
12s 7p SP	-24.52893	-37.68839	-54.40059	-74.80883	-99.40844	-128.54574
13s 7p	-24.52899	-37.68847	-54.40069	-74.80896	-99.40862	-128.54596
13s 8p SP	-24.52901	-37.68852	-54.40079	-74.80919	-99.40901	-128.54657
14s 8p	-	-	-	-	-	-128.54668
14s 9p SP	-	-	-	-	-	-128.54686
Hartree-Fock[b]	-24.529059	-37.688619	-54.400924	-74.809398	-99.409354	-128.54708

a) S = s-set exponents optimized. SP = both s and p-exponents optimized. These optimized exponents were used in constructing the basis sets where no optimization is indicated.

b) From Table 3.

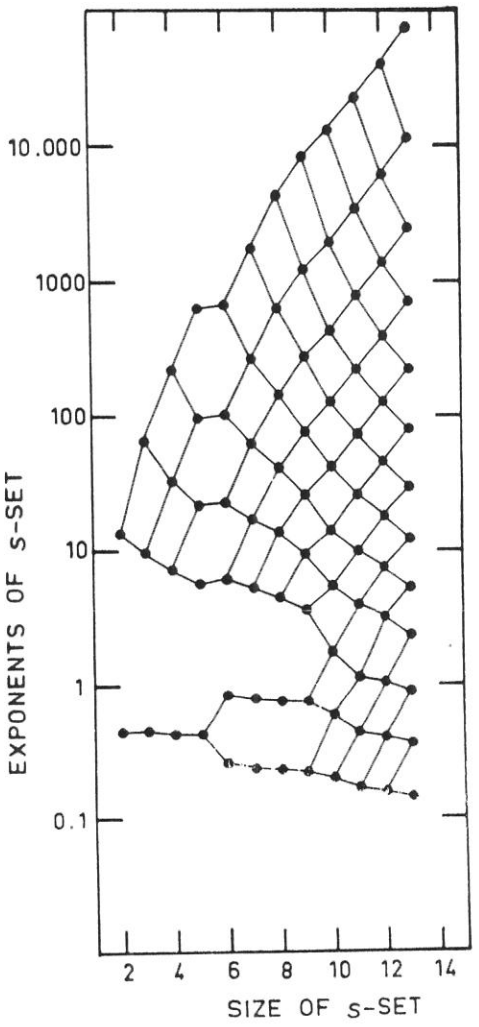

Fig. 1: Exponents of optimal sets of s-Gaussians for N(^{4}S). Connecting lines emphasize relationships between sets of different size.

CHARGE = 1.000000

VECTOR COUPLING COEFFICIENTS K

-1.00000000	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	

H(^{2}S)

HYDROGEN 2S SET

TOTAL HF ENERGY
-0.48581271520 00

POTENTIAL ENERGY -0.97163826260 00 KINETIC ENERGY 0.48582554740 00

VIRIAL THEOREM
-0.19999735870 01

HYDROGEN 3S SET

TOTAL HF ENERGY
-0.49697925130 00

POTENTIAL ENERGY -0.99396604960 00 KINETIC ENERGY 0.49698679830 00

VIRIAL THEOREM
-0.19999848150 01

HYDROGEN 4S SET

TOTAL HF ENERGY
-0.49927840470 00

POTENTIAL ENERGY -0.99855716760 00 KINETIC ENERGY 0.49927876290 00

VIRIAL THEOREM
-0.19999992830 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S	
1.0	0.201540
1.0	1.332699

S	
1.0	0.151398
1.0	0.681444
1.0	4.501800

S	
1.0	0.121953
1.0	0.444569
1.0	1.962496
1.0	13.013372

ORBITAL ENERGIES,EIGENVECTORS

-0.48531
0.821260
0.274370

-0.49698
0.647752
0.407826
0.070452

-0.49928
0.501131
0.478313
0.137952
0.019578

HYDROGEN 5S SET

TOTAL HF ENERGY
-0.4998098143D 00

POTENTIAL ENERGY	KINETIC ENERGY
-0.9996006482D 00	0.4997908339D 00

VIRIAL THEOREM
-0.2000037977D 01

HYDROGEN 6S SET

TOTAL HF ENERGY
-0.4999455671D 00

POTENTIAL ENERGY	KINETIC ENERGY
-0.9998909259D 00	0.4999453588D 00

VIRIAL THEOREM
-0.2000000417D 01

HYDROGEN 7S SET

TOTAL HF ENERGY
-0.4999832849D 00

POTENTIAL ENERGY	KINETIC ENERGY
-0.9999633148D 00	0.4999800299D 00

VIRIAL THEOREM
-0.2000006510D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

	S
1.0	0.102741
1.0	0.325840
1.0	1.158786
1.0	5.094798
1.0	33.865014

	S
1.0	0.089891
1.0	0.258053
1.0	0.797670
1.0	2.823854
1.0	12.409558
1.0	82.636374

	S
1.0	0.079891
1.0	0.212149
1.0	0.591063
1.0	1.815041
1.0	6.424830
1.0	28.276596
1.0	188.614448

ORBITAL ENERGIES,EIGENVECTORS

	-0.49981
	0.383568
	0.503709
	0.202846
	0.045316
	0.006068

	-0.49995
	0.296070
	0.497379
	0.256922
	0.075577
	0.015345
	0.002006

	-0.49998
	0.226499
	0.472522
	0.301057
	0.109381
	0.028433
	0.005551
	0.000718

HYDROGEN 8S SET

TOTAL HF ENERGY
-0.49999453410 00

POTENTIAL ENERGY	KINETIC ENERGY
-0.99999086350 00	0.49999632940 00

VIRIAL THEOREM
-0.19999964090 01

HYDROGEN 9S SET

TOTAL HF ENERGY
-0.49999809560 00

POTENTIAL ENERGY	KINETIC ENERGY
-0.99999551670 00	0.49999742110 00

VIRIAL THEOREM
-0.20000013490 01

HYDROGEN 10S SET

TOTAL HF ENERGY
-0.49999924360 00

POTENTIAL ENERGY	KINETIC ENERGY
-0.99999900040 00	0.49999975680 00

VIRIAL THEOREM
-0.19999989730 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

	S
1.0	0.072791
1.0	0.181120
1.0	0.465544
1.0	1.282709
1.0	3.904505
1.0	13.732173
1.0	60.241959
1.0	402.009948

	S
1.0	0.066180
1.0	0.155838
1.0	0.372145
1.0	0.938258
1.0	2.565036
1.0	7.825986
1.0	27.704222
1.0	123.524314
1.0	837.219740

	S
1.0	0.062157
1.0	0.138046
1.0	0.304802
1.0	0.710716
1.0	1.794924
1.0	4.915078
1.0	15.018344
1.0	54.698039
1.0	254.017712
1.0	1776.775559

ORBITAL ENERGIES,EIGENVECTORS

-0.49999
0.176456
0.436328
0.330883
0.142300
0.044899
0.011200
0.002165
0.000279

-0.50000
0.133721
0.391529
0.350387
0.178008
0.065862
0.019518
0.004737
0.000895
0.000112

-0.50000
0.107330
0.339658
0.352349
0.213239
0.090342
0.030540
0.008863
0.002094
0.000372
0.000044

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He(^{1}S)

CHARGE = 2.000000

VECTOR COUPLING COEFFICIENTS K

0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	

HELIUM 2S SET

TOTAL HF ENERGY
-0.27+7066120D 01

TENTIAL ENERGY KINETIC ENERGY
.5494227586D 01 0.2747161467D 01

VIRIAL THEOREM
-0.19999652930 01

HELIUM 3S SET

TOTAL HF ENERGY
-0.28356798680 01

POTENTIAL ENERGY KINETIC ENERGY
-0.5671405315D 01 0.2835725447D 01

VIRIAL THEOREM
-0.1999983927D 01

HELIUM 4S SET

TOTAL HF ENERGY
-0.28551604200 01

POTENTIAL ENERGY KINETIC ENERGY
-0.57104850170 01 0.2855324597D 01

VIRIAL THEOREM
-0.19999425020 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S	
1.0	0.532198
1.0	4.098394

S	
1.0	0.382993
1.0	1.999349
1.0	13.626736

S	
1.0	0.297964
1.0	1.241774
1.0	5.778030
1.0	38.421634

ORBITAL ENERGIES,EIGENVECTORS

-0.85890

0.925618
0.293141

-0.90357

0.657278
0.409143
0.080241

-0.91413

0.513586
0.469630
0.154679
0.023766

HELIUM 5S SET

TOTAL HF ENERGY
-0.28598954190 01

POTENTIAL ENERGY	KINETIC ENERGY
-0.57197850940 01	0.28598896750 01

VIRIAL THEOREM
-0.20000020080 01

S	
1.0	0.244564
1.0	0.874047
1.0	3.319825
1.0	14.768906
1.0	98.124267

-0.91687

	0.397445
	0.487488
	0.220765
	0.054836
	0.007576

HELIUM 6S SET

TOTAL HF ENERGY
-0.28611532970 01

POTENTIAL ENERGY	KINETIC ENERGY
-0.57222565410 01	0.28611032440 01

VIRIAL THEOREM
-0.20000174940 01

S	
1.0	0.208245
1.0	0.664349
1.0	2.202780
1.0	7.955702
1.0	35.022805
1.0	233.092501

-0.91763

	0.306262
	0.478261
	0.272853
	0.091421
	0.019628
	0.002600

HELIUM 7S SET

TOTAL HF ENERGY
-0.28615142200 01

POTENTIAL ENERGY	KINETIC ENERGY
-0.57230267370 01	0.28615125170 01

VIRIAL THEOREM
-0.20000005950 01

S	
1.0	0.183315
1.0	0.536241
1.0	1.607997
1.0	5.080905
1.0	18.036064
1.0	79.275179
1.0	528.390342

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

ORBITAL ENERGIES,EIGENVECTORS

-0.91735

	0.238915
	0.452874
	0.308474
	0.127832
	0.036011
	0.007219
	0.000940

HELIUM 8S SET

TOTAL HF ENERGY
-0.2861624827D 01

POTENTIAL ENERGY KINETIC ENERGY
-0.5723251434D 01 0.2861627007D 01

VIRIAL THEOREM
-0.1999999238D 01

HELIUM 9S SET

TOTAL HF ENERGY
-0.2861660624D 01

POTENTIAL ENERGY KINETIC ENERGY
-0.5723317545D 01 0.2861656921D 01

VIRIAL THEOREM
-0.2000001294D 01

HELIUM 10S SET

TOTAL HF ENERGY
-0.2861672938D 01

POTENTIAL ENERGY KINETIC ENERGY
-0.5723347820D 01 0.2861674882D 01

VIRIAL THEOREM
-0.1999999321D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S	
1.0	0.164206
1.0	0.447316
1.0	1.240443
1.0	3.364152
1.0	11.036173
1.0	39.080465
1.0	172.044569
1.0	1149.270536

S	
1.0	0.148805
1.0	0.385286
1.0	1.006248
1.0	2.686970
1.0	7.520262
1.0	23.100840
1.0	82.041904
1.0	356.153493
1.0	2290.081800

S	
1.0	0.138709
1.0	0.343643
1.0	0.849674
1.0	2.132879
1.0	5.526897
1.0	15.277787
1.0	46.636262
1.0	164.299706
1.0	723.108918
1.0	4840.888547

ORBITAL ENERGIES,EIGENVECTORS

-0.91792	-0.91794	-0.91795
0.186596	0.146082	0.119881
0.419480	0.385908	0.351965
0.331795	0.344387	0.346146
0.162104	0.190179	0.212006
0.055612	0.076258	0.096302
0.014256	0.023537	0.034249
0.002768	0.005739	0.009995
0.000357	0.001099	0.002422
	0.000149	0.000463
		0.000059

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Li(^{2}S)

CHARGE = 3.000000

VECTOR COUPLING COEFFICIENTS K

-1.0000000	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	

LITHIUM 4S SET

TOTAL HF ENERGY
-0.73769059520 01

POTENTIAL ENERGY -0.14753979460 02 KINETIC ENERGY 0.73770735050 01

VIRIAL THEOREM
-0.19999772870 01

LITHIUM 5S SET

TOTAL HF ENERGY
-0.74181813530 01

POTENTIAL ENERGY -0.14836411310 02 KINETIC ENERGY 0.74182299590 01

VIRIAL THEOREM
-0.19999934480 01

LITHIUM 6S SET

TOTAL HF ENERGY
-0.74278589990 01

POTENTIAL ENERGY -0.14855748050 02 KINETIC ENERGY 0.74278890550 01

VIRIAL THEOREM
-0.19999959540 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		S		S	
1.0	0.047743	1.0	0.047648	1.0	0.047795
1.0	1.051753	1.0	0.836433	1.0	0.705778
1.0	5.179275	1.0	3.303257	1.0	2.406806
1.0	34.882736	1.0	15.059103	1.0	8.907797
		1.0	100.000341	1.0	39.428548
				1.0	262.018797

ORBITAL ENERGIES,EIGENVECTORS

		-2.47020	-0.19497		
-2.44620	-0.19445			-2.47633	-0.19500
		0.016125	1.032647		
0.028554	1.026865	0.522270	-0.166712	0.010017	1.036505
0.658596	-0.189448	0.460220	-0.080387	0.416219	-0.145890
0.397200	-0.066754	0.142192	-0.022863	0.480180	-0.090853
0.073774	-0.012093	0.021172	-0.003273	0.202259	-0.032336
				0.047823	-0.007487
				0.006510	-0.000994

LITHIUM 7S SET

TOTAL HF ENERGY
-0.74293593009 01

POTENTIAL ENERGY -0.14853744544D 02 KINETIC ENERGY 0.74293852440 01

VIRIAL THEOREM
-0.1999996508D 01

LITHIUM 8S SET

TOTAL HF ENERGY
-0.7431751015D 01

POTENTIAL ENERGY -0.14863390869D 02 KINETIC ENERGY 0.74316396790 01

VIRIAL THEOREM
-0.2000014981D 01

LITHIUM 9S SET

TOTAL HF ENERGY
-0.74324133080 01

POTENTIAL ENERGY -0.1486443611D 02 KINETIC ENERGY 0.74320228010 01

VIRIAL THEOREM
-0.20000525440 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

	S
1.0	0.030339
1.0	0.075307
1.0	0.732905
1.0	2.491427
1.0	9.212495
1.0	40.760906
1.0	270.881090

	S
1.0	0.028116
1.0	0.072548
1.0	0.630596
1.0	1.921189
1.0	6.176662
1.0	22.082739
1.0	97.155099
1.0	647.083636

	S
1.0	0.028095
1.0	0.073968
1.0	0.542238
1.0	1.495542
1.0	4.286148
1.0	13.232594
1.0	46.549541
1.0	204.026470
1.0	1359.446605

ORBITAL ENERGIES, EIGENVECTORS

-2.47526	-0.19621
-0.010535	-0.577024
0.025089	-0.502659
0.426737	0.167085
0.472445	0.085543
0.195696	0.033242
0.045984	0.007232
0.006247	0.000994

-2.47702	-0.19630
-0.005375	-0.515129
0.014469	-0.572764
0.338834	0.150395
0.471834	0.092223
0.246890	0.042188
0.077505	0.012337
0.016164	0.002556
0.002125	0.000332

-2.47758	-0.19631
-0.002444	-0.521225
0.008132	-0.573351
0.255307	0.131809
0.450345	0.098292
0.294333	0.050977
0.117376	0.019108
0.032466	0.005124
0.006485	0.001017
0.000844	0.000132

LITHIUM 10S SET

TOTAL HF ENERGY
-0.7432572380D 01

POTENTIAL ENERGY -0.1466484751D 02 KINETIC ENERGY 0.7432275131D 01

VIRIAL THEOREM
-0.2000039994D 01

LITHIUM 11S SET

TOTAL HF ENERGY
-0.7432643290D 01

POTENTIAL ENERGY -0.1486509239D 02 KINETIC ENERGY 0.7432449100D 01

VIRIAL THEOREM
-0.2000026127D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S	
1.0	0.028927
1.0	0.076438
1.0	0.436688
1.0	1.023091
1.0	2.533132
1.0	6.843695
1.0	20.477806
1.0	71.215365
1.0	311.033717
1.0	2072.040929

S	
1.0	0.027778
1.0	0.074659
1.0	0.338768
1.0	0.704648
1.0	1.629594
1.0	4.084138
1.0	11.061892
1.0	33.377097
1.0	116.988551
1.0	513.280005
1.0	3427.557254

ORBITAL ENERGIES, EIGENVECTORS

-2.47764	-0.19631
-0.000940	-0.547278
0.004337	-0.552672
0.147087	0.096338
0.367598	0.103774
0.354530	0.064361
0.194447	0.033059
0.072206	0.011469
0.019392	0.003071
0.003842	0.000599
0.000499	0.000078

-2.47774	-0.19631
-0.000248	-0.518573
0.002236	-0.583000
0.063342	0.046469
0.267423	0.113144
0.382973	0.076445
0.268080	0.047867
0.124590	0.020118
0.041715	0.006680
0.010631	0.001658
0.002065	0.000324
0.000266	0.000042

LITHIUM 12S SET

TOTAL HF ENERGY
-0.74326d9615D 01

POTENTIAL ENERGY	KINETIC ENERGY
-0.14865392920 02	0.74327033040 01

VIRIAL THEOREM
-0.1999998158D 01

LITHIUM 13S SET

TOTAL HF ENERGY
-0.74327C9822D 01

POTENTIAL ENERGY	KINETIC ENERGY
-0.14865381890 02	0.74326720730 01

VIRIAL THEOREM
-0.2000005079D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S	
1.0	0.024311
1.0	0.055055
1.0	0.105971
1.0	0.479345
1.0	1.109366
1.0	2.653378
1.0	6.694067
1.0	18.213554
1.0	55.444215
1.0	195.155045
1.0	855.557147
1.0	5710.284999

S	
1.0	0.022468
1.0	0.051237
1.0	0.113995
1.0	0.362648
1.0	0.802261
1.0	1.831256
1.0	4.372801
1.0	11.017631
1.0	29.999891
1.0	91.124163
1.0	321.459939
1.0	1416.811212
1.0	9497.936395

ORBITAL ENERGIES, EIGENVECTORS

-2.47769	-0.19632
0.001822	-0.359311
-0.006231	-0.559781
0.011769	-0.185291
0.174607	0.115518
0.366807	0.091011
0.327643	0.061251
0.182426	0.030450
0.074431	0.012020
0.023021	0.003622
0.005663	0.000889
0.001092	0.000170
0.000141	0.000022

-2.47773	-0.19632
0.000258	-0.294720
0.000027	-0.613738
0.001969	-0.212187
0.086735	0.088567
0.303475	0.100370
0.357832	0.071944
0.239381	0.041589
0.114780	0.018768
0.042356	0.006740
0.012605	0.001981
0.003062	0.000479
0.000584	0.000091
0.000075	0.000012

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VECTOR COUPLING COEFFICIENTS K

0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	

BERYLLIUM 2S SET

TOTAL HF ENERGY
-0.1412004528D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.2824053226D 02	0.1412048697D 02

VIRIAL THEOREM
-0.1999968720D 01

BERYLLIUM 2S SET

TOTAL HF ENERGY
-0.1225014792D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.2450073460D 02	0.1225054168D 02

VIRIAL THEOREM
-0.1999971939D 01

BERYLLIUM 4S SET

TOTAL HF ENERGY
-0.1446789970D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.2893574654D 02	0.1446784685D 02

VIRIAL THEOREM
-0.2000003653D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S	
1.0	0.100128
1.0	3.869478

S	
1.0	0.102976
1.0	2.741442
1.0	19.445986

S	
1.0	0.103865
1.0	2.050391
1.0	9.851535
1.0	66.022855

ORBITAL ENERGIES,EIGENVECTORS

-3.65202	-0.25601
0.126006	1.007842
0.970147	-0.301065

-4.50596	-0.29437
0.055153	1.022117
0.817817	-0.231546
0.268022	-0.052173

-4.68159	-0.29992
0.029547	1.030560
0.662124	-0.199164
0.391286	-0.077823
0.070864	-0.012785

BERYLLIUM 5S SET

TOTAL HF ENERGY
-0.14539859200 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.29079891430 02	0.14540032230 02

VIRIAL THEOREM
-0.19999881000 01

BERYLLIUM 6S SET

TOTAL HF ENERGY
-0.14551588890 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.29107757220 02	0.14556168340 02

VIRIAL THEOREM
-0.19999685950 01

BERYLLIUM 7S SET

TOTAL HF ENERGY
-0.14567244530 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.29134620360 02	0.14567375830 02

VIRIAL THEOREM
-0.19999909860 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S	
1.0	0.104444
1.0	1.661636
1.0	6.413151
1.0	28.966257
1.0	192.256800

S	
1.0	0.067376
1.0	0.198210
1.0	1.767558
1.0	6.819528
1.0	30.827597
1.0	204.906144

S	
1.0	0.060022
1.0	0.180274
1.0	1.469242
1.0	4.897471
1.0	17.920402
1.0	79.156167
1.0	526.200598

ORBITAL ENERGIES,EIGENVECTORS.

-4.72093	-0.30068
0.017691	1.035575
0.532341	-0.169866
0.451978	-0.097803
0.135371	-0.024240
0.019826	-0.003572

-4.71931	-0.30821
-0.018105	-0.684448
0.048086	-0.406007
0.545583	0.199137
0.434625	0.091120
0.126404	0.024353
0.018353	0.003375

-4.72917	-0.30891
-0.009471	-0.590306
0.026791	-0.511665
0.438757	0.174192
0.465966	0.105570
0.186104	0.035884
0.042702	0.007923
0.005764	0.001052

BERYLLIUM 8S SET

TOTAL HF ENERGY
-0.14571235780 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.29142498C8D 02	0.1457125231D 02

VIRIAL THEOREM
-0.19999988660 01

BERYLLIUM 9S SET

TOTAL HF ENERGY
-0.1457233014D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.2914459567D 02	0.1457226552D 02

VIRIAL THEOREM
-0.2000204434D 01

BERYLLIUM 10 S SET

TOTAL HF ENERGY
-0.1457258283D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.2914511430D 02	0.1457253147D 02

VIRIAL THEOREM
-0.2000003524D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S	
1.0	0.059132
1.0	0.180437
1.0	1.288293
1.0	3.859128
1.0	12.278640
1.0	43.789227
1.0	192.594655
1.0	1282.784656

S	
1.0	0.059170
1.0	0.181732
1.0	1.132424
1.0	3.056264
1.0	8.629560
1.0	26.587957
1.0	93.672648
1.0	410.319811
1.0	2732.328145

S	
1.0	0.052876
1.0	0.152802
1.0	0.395917
1.0	1.369672
1.0	3.733798
1.0	10.697123
1.0	33.234901
1.0	117.930588
1.0	519.359716
1.0	3466.566460

ORBITAL ENERGIES,EIGENVECTORS

-4.73165	-0.30901
-0.005721	-0.581686
0.017730	-0.525950
0.358014	0.153138
0.466518	0.114578
0.233521	0.045536
0.070748	0.013370
0.014572	0.002649
0.001909	0.000350

-4.73225	-0.30901
-0.003524	-0.582939
0.011920	-0.528229
0.280567	0.126478
0.446089	0.121907
0.280109	0.055624
0.107092	0.020745
0.028888	0.005251
0.005724	0.001056
0.000745	0.000135

-4.73235	-0.30919
0.001757	-0.481108
-0.007749	-0.587916
0.038127	-0.040613
0.345172	0.157834
0.431841	0.102203
0.237493	0.048186
0.C34640	0.015853
0.021982	0.004068
0.004286	0.000780
0.000554	0.000101

BERYLLIUM 11s SET

TOTAL HF ENERGY
-0.14572668270 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.29145593120 02	0.14572724850 02

VIRIAL THEOREM
-0.20000098420 01

BERYLLIUM 12S SET

TOTAL HF ENERGY
-0.14572952300 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.29145712040 02	0.14572759750 02

VIRIAL THEOREM
-0.20000132130 01

BERYLLIUM 13S SET

TOTAL HF ENERGY
-0.14572987960 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.29145943430 02	0.14572955470 0

VIRIAL THEOREM
-0.20000022290 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S	
1.0	0.043664
1.0	0.109943
1.0	0.261124
1.0	1.088105
1.0	2.727345
1.0	7.083735
1.0	19.697209
1.0	60.235140
1.0	212.556498
1.0	936.508212
1.0	6264.728780

S	
1.0	0.043102
1.0	0.106756
1.0	0.258705
1.0	0.830394
1.0	1.967869
1.0	4.864860
1.0	12.721647
1.0	35.824670
1.0	111.638010
1.0	398.403613
1.0	1760.979495
1.0	11781.668696

S	
1.0	0.042427
1.0	0.104176
1.0	0.257696
1.0	0.608615
1.0	1.452144
1.0	3.460891
1.0	8.721372
1.0	23.372177
1.0	67.223469
1.0	211.740476
1.0	760.358486
1.0	3372.318148
1.0	22631.589258

ORBITAL ENERGIES,EIGENVECTORS

-4.73258	-0.30926
0.001597	-0.313328
-0.006123	-0.585362
0.016293	-0.226711
0.244876	0.129636
0.417889	0.115569
0.296200	0.061726
0.131710	0.025505
0.042616	0.007888
0.010700	0.001966
0.002062	0.000375
0.000265	0.000048

-4.73265	-0.30926
0.000063	-0.301560
-0.000433	-0.578335
0.003709	-0.255017
0.138194	0.089616
0.380352	0.129431
0.351851	0.077629
0.186700	0.037324
0.070838	0.013235
0.020723	0.003836
0.004951	0.000901
0.000939	0.000172
0.000120	0.000022

-4.73264	-0.30926
-0.000230	-0.287668
0.000912	-0.531647
-0.002125	-0.272441
0.066401	0.053005
0.309229	0.131620
0.386776	0.094988
0.246099	0.050521
0.105837	0.020199
0.034842	0.006466
0.009558	0.001750
0.002227	0.000407
0.000618	0.000076
0.000053	0.000010

CHARGE = 5.000000

VECTOR COUPLING COEFFICIENTS K

0.0	0.0	-1.66666667	0.13333333	0.0
0.0	0.0	0.0	0.0	0.0

B(^{2}P)

BORON 4/3 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.24336119[illegible]D 02

POTENTIAL ENERGY -0.48673517[illegible]D 02 KINETIC ENERGY 0.24337398070 02

VIRIAL THEOREM
-0.19999474510 01

BORON 5/2 SOURCE SET

TOTAL HF ENERGY
-0.24447263130 02

POTENTIAL ENERGY -0.48894655720 02 KINETIC ENERGY 0.24447392580 02

VIRIAL THEOREM
-0.19999947050 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.189977	2.0	0.168230
1.0	3.379772	2.0	0.924520
1.0	16.007033		
1.0	106.949418		

S		P	
1.0	0.190443	2.0	0.168225
1.0	2.746303	2.0	0.924518
1.0	10.450108		
1.0	46.924962		
1.0	311.324130		

ORBITAL ENERGIES,EIGENVECTORS

-7.63187	-0.47787	-0.27449
0.032968	1.034928	0.809935
0.663270	-0.212940	0.328902
0.367633	-0.097386	0.0
0.069252	-0.013701	0.0

-7.69071	-0.47883	-0.27595
0.020275	-1.039661	0.808602
0.534311	0.177304	0.330758
0.449123	0.111617	0.0
0.132898	0.026106	0.0
0.019305	0.003867	0.0

BORON 6/2 DERIVED SET

TOTAL HF ENERGY
-0.24471773570 02

POTENTIAL ENERGY KINETIC ENERGY
-0.48944590850 02 0.24472817280 02

VIRIAL THEOREM
-0.19999573520 01

BORON 5/3 DERIVED SET

TOTAL HF ENERGY
-0.24466173590 02

POTENTIAL ENERGY KINETIC ENERGY
-0.48939859980 02 0.24473686290 02

VIRIAL THEOREM
-0.19996930290 01

A-19

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.117860	2.0	0.168230
1.0	0.362570	2.0	0.924520
1.0	2.316030		
1.0	11.071000		
1.0	49.681900		
1.0	329.769000		

S		P	
1.0	0.190440	2.0	0.123310
1.0	2.746300	2.0	0.518270
1.0	10.450100	2.0	2.577170
1.0	46.925000		
1.0	311.324000		

ORBITAL ENERGIES,EIGENVECTORS

-7.68997	-0.49306	-0.28319
-0.017087	-0.668395	0.808447
0.050727	-0.433712	0.330969
0.544846	0.212676	0.0
0.432330	0.103222	0.0
0.124541	0.026388	0.0
0.018002	0.003681	0.0

-7.67766	-0.47788	-0.29490
0.020480	-1.039718	0.632813
0.534591	0.177749	0.456266
0.448803	0.111457	0.106074
0.132883	0.026137	0.0
0.019298	0.003886	0.0

BORON 6/3 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.24490779180 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.48981669220 02	0.24490890040 02

VIRIAL THEOREM
-0.19999954730 01

BORON 7/3 SOURCE SET

TOTAL HF ENERGY
-0.24514460210 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.49028974910 02	0.24514514700 02

VIRIAL THEOREM
-0.19999977770 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.117864	2.0	0.123310
1.0	0.362568	2.0	0.518270
1.0	2.916034	2.0	2.577170
1.0	11.071020		
1.0	49.681859		
1.0	329.769363		

S		P	
1.0	0.107892	2.0	0.123306
1.0	0.338409	2.0	0.518268
1.0	2.450751	2.0	2.577167
1.0	8.064844		
1.0	29.285383		
1.0	129.186744		
1.0	858.893333		

ORBITAL ENERGIES, EIGENVECTORS

-7.67902	-0.49257	-0.30284
-0.017208	-0.671368	0.632794
0.051124	-0.430341	0.456396
0.544993	0.212392	0.105837
0.432048	0.102972	0.0
0.124523	0.026359	0.0
0.017996	0.003675	0.0

-7.69223	-0.49339	-0.30350
-0.009466	-0.603551	0.632004
0.030764	-0.508673	0.457137
0.443289	0.184407	0.106032
0.461774	0.119137	0.0
0.181837	0.038700	0.0
0.041258	0.008528	0.0
0.005553	0.001119	0.0

BORON 8/3 DERIVED SET

TOTAL HF ENERGY
-0.24520511220 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.49040911730 02	0.24520400510 02

VIRIAL THEOREM
-0.20000045150 01

BORON 7/4 DERIVED SET

TOTAL HF ENERGY
-0.24518814480 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.49038093100 02	0.24519278620 02

VIRIAL THEOREM
-0.19999810710 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.105550	2.0	0.123310
1.0	0.334990	2.0	0.518270
1.0	2.143660	2.0	2.577170
1.0	6.335320		
1.0	19.970400		
1.0	71.005900		
1.0	311.957000		
1.0	2076.990000		

S		P	
1.0	0.107890	2.0	0.095600
1.0	0.338410	2.0	0.337560
1.0	2.450750	2.0	1.245750
1.0	8.064840	2.0	6.028140
1.0	29.285400		
1.0	129.187000		
1.0	858.893000		

ORBITAL ENERGIES, EIGENVECTORS

-7.09568	-0.49352	-0.30369
-0.005716	-0.588526	0.631735
0.020773	-0.528925	0.457382
0.361298	0.158445	0.106101
0.463839	0.130275	0.0
0.230393	0.049703	0.0
0.069025	0.014557	0.0
0.014175	0.002846	0.0
0.001856	0.000378	0.0

-7.69050	-0.49373	-0.30794
-0.009486	-0.603892	0.481249
0.030829	-0.508321	0.504505
0.443345	0.184479	0.197149
0.461712	0.119048	0.035252
0.181822	0.038700	0.0
0.041255	0.008524	0.0
0.005552	0.001119	0.0

IBM Research

GAUSSIAN BASIS SETS FOR THE ATOMS H-Ne FOR USE IN MOLECULAR CALCULATIONS

F. B. van Duijneveldt

December 10, 1971

RJ 945

Yorktown Heights, New York

San José, California

Zurich, Switzerland

BORON 8/4 SOURCE SET

TOTAL HF ENERGY
-0.24524967930 02

POTENTIAL ENERGY KINETIC ENERGY
-0.49049961730 02 0.24525093800 02

VIRIAL THEOREM
-0.19999907900 01

BORON 9/4 DERIVED SET

TOTAL HF ENERGY
-0.24526493840 02

POTENTIAL ENERGY KINETIC ENERGY
-0.49051736350 02 0.24525242510 02

VIRIAL THEOREM
-0.20000510220 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.105546	2.0	0.095596
1.0	0.334987	2.0	0.337561
1.0	2.143664	2.0	1.245748
1.0	6.335321	2.0	6.028137
1.0	19.970448		
1.0	71.005879		
1.0	311.957177		
1.0	2076.992197		

S		P	
1.0	0.103710	2.0	0.095600
1.0	0.331110	2.0	0.337560
1.0	1.751270	2.0	1.245750
1.0	4.524440	2.0	6.028140
1.0	12.328800		
1.0	37.055500		
1.0	128.747000		
1.0	561.198000		
1.0	3733.330000		

ORBITAL ENERGIES,EIGENVECTORS

-7.69395	-0.49386	-0.30814
-0.005731	-0.588843	0.480949
0.020828	-0.528611	0.504695
0.361369	0.158553	0.197270
0.463779	0.130170	0.035276
0.230371	0.049699	0.0
0.069070	0.014552	0.0
0.014174	0.002846	0.0
0.001856	0.000377	0.0

-7.69489	-0.49394	-0.30827
-0.002457	-0.576218	0.480794
0.011064	-0.544841	0.504787
0.246825	0.112641	0.197330
0.437282	0.144548	0.035284
0.300099	0.067025	0.0
0.121457	0.026490	0.0
0.034060	0.006857	0.0
0.006852	0.001405	0.0
0.000895	0.000179	0.0

BORON 9/5 SOURCE SET

TOTAL HF ENERGY
-0.24527473630 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.49053727470 02	0.24526253840 02

VIRIAL THEOREM
-0.20000497340 01

BORON 10/5 DERIVED SET

TOTAL HF ENERGY
-0.24528083600 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.49056539530 02	0.24528455930 02

VIRIAL THEOREM
-0.19999848200 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.103714	2.0	0.077877
1.0	0.331106	2.0	0.241978
1.0	1.751267	2.0	0.760671
1.0	4.524435	2.0	2.655995
1.0	12.328842	2.0	12.363854
1.0	37.055525		
1.0	128.746549		
1.0	561.197732		
1.0	3733.332716		

S		P	
1.0	0.094020	2.0	0.077880
1.0	0.283690	2.0	0.241980
1.0	0.825630	2.0	0.760670
1.0	2.476990	2.0	2.656000
1.0	6.698250	2.0	12.363900
1.0	19.102400		
1.0	59.187600		
1.0	209.557000		
1.0	921.456000		
1.0	6149.230000		

ORBITAL ENERGIES,EIGENVECTORS

-7.69472	-0.49415	-0.30924
-0.002458	-0.576199	0.359281
0.011070	-0.544869	0.504219
0.246847	0.112681	0.273278
0.437267	0.144529	0.078312
0.300097	0.067030	0.012741
0.121453	0.026488	0.0
0.034060	0.006857	0.0
0.006852	0.001405	0.0
0.000895	0.000179	0.0

-7.69478	-0.49439	-0.30941
0.001460	-0.489142	0.359226
-0.005147	-0.595312	0.504264
0.055944	-0.030150	0.273275
0.371713	0.173223	0.078311
0.418148	0.108286	0.012740
0.216546	0.048745	0.0
0.074494	0.015415	0.0
0.019099	0.003920	0.0
0.003719	0.000749	0.0
0.000480	0.000097	0.0

BORON 10/6 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.24528310770 02

POTENTIAL ENERGY KINETIC ENERGY
-0.49056791860 02 0.24528481090 02

VIRIAL THEOREM
-0.19999930560 01

BORON 11/6 SOURCE SET

TOTAL HF ENERGY
-0.24528733170 02

POTENTIAL ENERGY KINETIC ENERGY
-0.49056911990 02 0.24528178820 02

VIRIAL THEOREM
-0.20000226010 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.094022	2.0	0.062300
1.0	0.283686	2.0	0.170740
1.0	0.825626	2.0	0.474150
1.0	2.476991	2.0	1.388700
1.0	6.698251	2.0	4.684150
1.0	19.102357	2.0	20.816100
1.0	59.187598		
1.0	209.557154		
1.0	921.455904		
1.0	6149.230249		

S		P	
1.0	0.075823	2.0	0.062303
1.0	0.195822	2.0	0.170739
1.0	0.485398	2.0	0.474153
1.0	1.726348	2.0	1.388704
1.0	4.281016	2.0	4.684146
1.0	11.162879	2.0	20.816050
1.0	31.467297		
1.0	97.963272		
1.0	350.221898		
1.0	1549.989006		
1.0	10370.398158		

ORBITAL ENERGIES,EIGENVECTORS

-7.69488	-0.49452	-0.30962
0.001461	-0.489065	0.237954
-0.005148	-0.595390	0.463938
0.055946	-0.030148	0.346173
0.371716	0.173234	0.142401
0.418145	0.108288	0.036610
0.216546	0.048748	0.005714
0.074495	0.015416	0.0
0.019099	0.003920	0.0
0.003719	0.000749	0.0
0.000480	0.000097	0.0

-7.69524	-0.49466	-0.30975
0.000918	-0.307782	0.237964
-0.003281	-0.586686	0.463871
0.014809	-0.245831	0.346228
0.227919	0.126467	0.142407
0.421434	0.135384	0.036615
0.306284	0.071700	0.005714
0.133872	0.028920	0.0
0.042003	0.008611	0.0
0.010256	0.002091	0.0
0.001952	0.000394	0.0
0.000250	0.000051	0.0

BORON 12/6 DERIVED SET

TOTAL HF ENERGY
-0.24528873610 02

POTENTIAL ENERGY -0.49057336040 02 KINETIC ENERGY 0.24528462440 02

VIRIAL THEOREM
-0.20000167630 01

BORON 11/7 DERIVED SET

TOTAL HF ENERGY
-0.24528789760 02

POTENTIAL ENERGY -0.49057059900 02 KINETIC ENERGY 0.24528270150 02

VIRIAL THEOREM
-0.20000211840 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.069600	2.0	0.062300
1.0	0.176790	2.0	0.170740
1.0	0.446360	2.0	0.474150
1.0	1.378840	2.0	1.388700
1.0	3.219160	2.0	4.684150
1.0	7.855100	2.0	20.816100
1.0	20.407100		
1.0	57.067400		
1.0	176.149000		
1.0	624.869000		
1.0	2756.590000		
1.0	18465.600000		

S		P	
1.0	0.075820	2.0	0.052490
1.0	0.195820	2.0	0.133180
1.0	0.485400	2.0	0.335620
1.0	1.726350	2.0	0.871830
1.0	4.281020	2.0	2.474800
1.0	11.162880	2.0	8.194620
1.0	31.467300	2.0	35.347300
1.0	97.963300		
1.0	350.222000		
1.0	1549.990000		
1.0	10370.400000		

ORBITAL ENERGIES, EIGENVECTORS

-7.69534	-0.49468	-0.30978
0.000174	-0.253125	0.237971
-0.000388	-0.586080	0.463847
0.005348	-0.304120	0.346250
0.139439	0.082286	0.142409
0.376525	0.144252	0.036617
0.352236	0.087800	0.005714
0.146172	0.041539	0.0
0.070118	0.014554	0.0
0.020686	0.004246	0.0
0.004997	0.001008	0.0
0.000952	0.000193	0.0
0.000122	0.000025	0.0

-7.69523	-0.49468	-0.30981
0.000918	-0.307754	0.162287
-0.003281	-0.586722	0.406985
0.014809	-0.245822	0.373068
0.227920	0.126468	0.203177
0.421433	0.135384	0.069980
0.306283	0.071699	0.016922
0.133872	0.028920	0.002416
0.042004	0.008611	0.0
0.010256	0.002091	0.0
0.001952	0.000394	0.0
0.000250	0.000051	0.0

BORON 12/7 SOURCE SET

TOTAL HF ENERGY
-0.2452893013D 02

POTENTIAL ENERGY KINETIC ENERGY
-0.4905748204D 02 0.2452855191D 02

VIRIAL THEOREM
-0.2000015420D 01

BORON 13/7 DERIVED SET

TOTAL HF ENERGY
-0.2452899054D 02

POTENTIAL ENERGY KINETIC ENERGY
-0.4905784151D 02 0.2452885097D 02

VIRIAL THEOREM
-0.2000005690D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.069603	2.0	0.052489
1.0	0.176793	2.0	0.133179
1.0	0.446363	2.0	0.335622
1.0	1.378844	2.0	0.871826
1.0	3.219158	2.0	2.474799
1.0	7.855098	2.0	8.194616
1.0	20.407073	2.0	35.347305
1.0	57.067411		
1.0	176.149194		
1.0	624.889488		
1.0	2756.588483		
1.0	18465.553973		

S		P	
1.0	0.068540	2.0	0.052490
1.0	0.169630	2.0	0.133180
1.0	0.421550	2.0	0.335620
1.0	1.114200	2.0	0.871830
1.0	2.496270	2.0	2.474800
1.0	5.741160	2.0	8.194620
1.0	13.971400	2.0	35.347300
1.0	36.295900		
1.0	102.007000		
1.0	316.491000		
1.0	1125.640000		
1.0	4972.100000		
1.0	33360.200000		

ORBITAL ENERGIES, EIGENVECTORS

-7.69533	-0.49470	-0.30984
0.000174	-0.253133	0.162325
-0.000388	-0.596076	0.406919
0.005348	-0.304115	0.373112
0.139441	0.082289	0.203168
0.376524	0.144251	0.069986
0.352237	0.087800	0.016922
0.186172	0.041539	0.002416
0.070118	0.014554	0.0
0.020685	0.004246	0.0
0.004997	0.001008	0.0
0.000952	0.000193	0.0
0.000122	0.000025	0.0

-7.69533	-0.49470	-0.30983
-0.000010	-0.238508	0.162303
0.000395	-0.570221	0.406954
0.001500	-0.329284	0.373088
0.078454	0.039027	0.203175
0.307938	0.141348	0.069982
0.373406	0.102450	0.016922
0.239568	0.055324	0.002416
0.105950	0.022472	0.0
0.036092	0.007452	0.0
0.010161	0.002060	0.0
0.002409	0.000488	0.0
0.000456	0.000092	0.0
0.000058	0.000012	0.0

BJRGN 13/8 SOURCE SET

TOTAL HF ENERGY
-0.24529005C8D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.49057907030 02	0.24528901950 02

VIRIAL THEOREM
-0.20000042040 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.063535	2.0	0.047648
1.0	0.159633	2.0	0.111151
1.0	0.421549	2.0	0.255634
1.0	1.114202	2.0	0.602136
1.0	2.496268	2.0	1.481256
1.0	5.741156	2.0	4.135394
1.0	13.971410	2.0	13.366101
1.0	36.295873	2.0	55.000000
1.0	102.007256		
1.0	316.491356		
1.0	1125.641723		
1.0	4972.095217		
1.0	33360.216573		

ORBITAL ENERGIES, EIGENVECTORS

-7.69531	-0.49470	-0.30984
-0.000010	-0.238499	0.121395
0.000395	-0.570252	0.340403
0.001500	-0.329255	0.371013
0.078455	0.039015	0.245583
0.307937	0.141355	0.111514
0.373607	0.102447	0.035983
0.239567	0.055325	0.008162
0.105950	0.022472	0.001124
0.036092	0.007452	0.0
0.010161	0.002060	0.0
0.002409	0.000488	0.0
0.000458	0.000093	0.0
0.000058	0.000012	0.0

CHARGE = 6.000000

VECTOR COUPLING COEFFICIENTS K

0.0	0.0	-0.66666667	-0.06666667	0.0	0.0
0.0	0.0	0.0	0.0	0.0	

C(^{3}P)

CARBON 4/2 DERIVED SOURCE SET

VIRIAL THEOREM
-0.19998724970 01

POTENTIAL ENERGY	KINETIC ENERGY
-0.74716245010 02	0.37360504290 02

TOTAL HF ENERGY
-0.37355740720 02

CARBON 5/2 SOURCE SET

TOTAL HF ENERGY
-0.37515253270 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.75036997030 02	0.37515743760 02

VIRIAL THEOREM
-0.19999869260 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.296721	2.0	0.279900
1.0	5.027480	2.0	1.560350
1.0	23.597440		
1.0	157.342970		

S		P	
1.0	0.296830	2.0	0.279901
1.0	4.081633	2.0	1.560346
1.0	15.385241		
1.0	68.797136		
1.0	456.243411		

ORBITAL ENERGIES,EIGENVECTORS

-11.24561	-0.67625	-0.37481
0.035091	1.037038	0.806007
0.663514	-0.219255	0.336481
0.385819	-0.093034	0.0
0.068377	-0.014179	0.0

-11.32839	-0.67755	-0.37675
0.021834	-1.041427	0.804999
0.533785	0.179209	0.337873
0.448479	0.120196	0.0
0.132078	0.027206	0.0
0.019102	0.004078	0.0

CARBON 5/3 DERIVED SET

TOTAL HF ENERGY
-0.37581160630 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.75177267070 02	0.37596106450 02

VIRIAL THEOREM
-0.19996024640 01

CARBON 6/3 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.37622965670 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.75245980660 02	0.37623015000 02

VIRIAL THEOREM
-0.19999986890 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.296830	2.0	0.199770
1.0	4.081630	2.0	0.854050
1.0	15.385200	2.0	4.187350
1.0	68.797100		
1.0	456.243000		

S		P	
1.0	0.181844	2.0	0.199770
1.0	0.577490	2.0	0.854050
1.0	4.367720	2.0	4.187350
1.0	16.461765		
1.0	73.640524		
1.0	488.726826		

ORBITAL ENERGIES,EIGENVECTORS

-11.30057	-0.67760	-0.41017
0.022174	-1.041533	0.624552
0.534311	0.179988	0.464227
0.447888	0.119918	0.111979
0.132046	0.027259	0.0
0.019090	0.004077	0.0

-11.30412	-0.70096	-0.42080
-0.016851	-0.676876	0.624307
0.054295	-0.430701	0.464575
0.546836	0.219723	0.111782
0.428730	0.109208	0.0
0.122190	0.027203	0.0
0.017563	0.003790	0.0

CARBON 7/3 SOURCE SET

TOTAL HF ENERGY
-0.3765651684D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.75312844550 02	0.37656327700 02

VIRIAL THEOREM
-0.20000050230 01

CARBON 8/3 DERIVED SET

TOTAL HF ENERGY
-0.3766512201D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.7532932753D 02	0.3766420552D 02

VIRIAL THEOREM
-0.2000024333D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.167130	2.0	0.199770
1.0	0.539158	2.0	0.854053
1.0	3.663116	2.0	4.187345
1.0	11.964903		
1.0	43.247698		
1.0	190.603978		
1.0	1267.163972		

S		P	
1.0	0.162070	2.0	0.199770
1.0	0.528300	2.0	0.854050
1.0	3.188800	2.0	4.187350
1.0	9.360540		
1.0	29.356300		
1.0	104.196000		
1.0	457.687000		
1.0	3047.420000		

ORBITAL ENERGIES,EIGENVECTORS

-11.32194	-0.70210	-0.42154
-0.009267	-0.613125	0.623756
0.033148	-0.504860	0.465078
0.444594	0.188777	0.111922
0.460002	0.127219	0.0
0.179789	0.040322	0.0
0.040526	0.008864	0.0
0.005446	0.001156	0.0

-11.32677	-0.70233	-0.42184
-0.005463	-0.591708	0.623531
0.022279	-0.531272	0.465284
0.360811	0.159137	0.111978
0.463532	0.139983	0.0
0.229521	0.052262	0.0
0.068341	0.015266	0.0
0.014007	0.002962	0.0
0.001833	0.000394	0.0

CARBON 7/4 DERIVED SET

TOTAL HF ENERGY
-0.3767132089D 02

POTENTIAL ENERGY KINETIC ENERGY
-0.7534356718D 02 0.3767224629D 02

VIRIAL THEOREM
-0.1999975435D 01

CARBON 8/4 SOURCE SET

TOTAL HF ENERGY
-0.3767993792D 02

POTENTIAL ENERGY KINETIC ENERGY
-0.7535989844D 02 0.3767996053D 02

VIRIAL THEOREM
-0.1999999400D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.167130	2.0	0.151970
1.0	0.539160	2.0	0.546940
1.0	3.663120	2.0	2.006580
1.0	11.964900	2.0	9.464520
1.0	43.247700		
1.0	190.604000		
1.0	1267.180000		

S		P	
1.0	0.162074	2.0	0.151974
1.0	0.528295	2.0	0.546943
1.0	3.188803	2.0	2.006582
1.0	9.360538	2.0	9.464518
1.0	29.356261		
1.0	104.195924		
1.0	457.687168		
1.0	3047.421082		

ORBITAL ENERGIES,EIGENVECTORS

-11.31869	-0.70355	-0.42978
-0.009299	-0.613384	0.470140
0.033255	-0.504613	0.507957
0.444693	0.188947	0.208839
0.459894	0.127099	0.037960
0.179761	0.040327	0.0
0.040521	0.008861	0.0
0.005446	0.001156	0.0

-11.32347	-0.70378	-0.43008
-0.005487	-0.591949	0.469896
0.022366	-0.531059	0.508099
0.360938	0.159349	0.208938
0.463426	0.139848	0.037978
0.229482	0.052261	0.0
0.068332	0.015262	0.0
0.014005	0.002962	0.0
0.001832	0.000394	0.0

CARBON 9/4 DERIVED SET

TOTAL HF ENERGY
-0.37682240640 02

POTENTIAL ENERGY KINETIC ENERGY
-0.75362011790 02 0.37679771140 02

VIRIAL THEOREM
-0.20000655390 01

CARBON 9/5 SOURCE SET

TOTAL HF ENERGY
-0.37685549160 02

POTENTIAL ENERGY KINETIC ENERGY
-0.75368603510 02 0.37683054340 02

VIRIAL THEOREM
-0.20000662050 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.156590	2.0	0.151970
1.0	0.511900	2.0	0.546940
1.0	2.403980	2.0	2.006580
1.0	6.143620	2.0	9.464520
1.0	16.787600		
1.0	50.877900		
1.0	178.073000		
1.0	778.756000		
1.0	5182.950000		

S		P	
1.0	0.156590	2.0	0.121940
1.0	0.511900	2.0	0.385540
1.0	2.418049	2.0	1.206710
1.0	6.175776	2.0	4.159240
1.0	16.823562	2.0	18.841800
1.0	50.815942		
1.0	178.350830		
1.0	782.204795		
1.0	5240.635258		

ORBITAL ENERGIES.EIGENVECTORS

-11.32472	-0.70397	-0.43034
-0.001324	-0.566667	0.469744
0.008778	-0.558699	0.508201
0.212656	0.091887	0.208990
0.439538	0.162452	0.037985
0.320724	0.077099	0.0
0.130519	0.030213	0.0
0.036293	0.007724	0.0
0.007256	0.001571	0.0
0.000947	0.000200	0.0

-11.32456	-0.70465	-0.43233
-0.001396	-0.566565	0.346861
0.009027	-0.558791	0.499411
0.214974	0.093012	0.288744
0.438742	0.161815	0.086279
0.318931	0.076607	0.013887
0.130600	0.030238	0.0
0.036344	0.007736	0.0
0.007228	0.001564	0.0
0.000937	0.000198	0.0

CARBON 10/5 DERIVED SET

TOTAL HF ENERGY
-0.3768665166D 02

POTENTIAL ENERGY -0.7537410553D 02 KINETIC ENERGY 0.3768745387D 02

VIRIAL THEOREM
-0.1999978714D 01

CARBON 10/6 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.3768741548D 02

POTENTIAL ENERGY -0.7537500438D 02 KINETIC ENERGY 0.3768758890D 02

VIRIAL THEOREM
-0.1999995399D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.134280	2.0	0.121940
1.0	0.393720	2.0	0.385540
1.0	1.017480	2.0	1.206710
1.0	3.486330	2.0	4.159240
1.0	9.493350	2.0	18.841800
1.0	27.133700		
1.0	84.338800		
1.0	299.519000		
1.0	1319.280000		
1.0	8806.650000		

S		P	
1.0	0.134271	2.0	0.095840
1.0	0.393724	2.0	0.274840
1.0	1.017479	2.0	0.772810
1.0	3.486330	2.0	2.239240
1.0	9.493353	2.0	7.472610
1.0	27.133675	2.0	32.692100
1.0	84.338836		
1.0	299.518755		
1.0	1319.281981		
1.0	8806.653419		

ORBITAL ENERGIES,EIGENVECTORS

-11.32468	-0.70507	-0.43251
0.002238	-0.432114	0.346831
-0.008304	-0.602725	0.499452
0.046632	-0.095503	0.288729
0.362670	0.176100	0.086270
0.428376	0.121981	0.013886
0.223743	0.053081	0.0
0.076551	0.016864	0.0
0.019525	0.004211	0.0
0.003787	0.000808	0.0
0.000489	0.000104	0.0

-11.32503	-0.70549	-0.43307
0.002239	-0.431929	0.230915
-0.008306	-0.602929	0.462755
0.046637	-0.095486	0.351437
0.362673	0.176118	0.151007
0.428373	0.121989	0.039116
0.223741	0.053087	0.005869
0.076551	0.016865	0.0
0.019524	0.004212	0.0
0.003787	0.000808	0.0
0.000489	0.000104	0.0

CARBON 11/6 SOURCE SET

TOTAL HF ENERGY
-0.37688020140 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.75375258250 02	0.37687238110 02

VIRIAL THEOREM
-0.20000207510 01

CARBON 12/6 DERIVED SET

TOTAL HF ENERGY
-0.37688203210 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.75375599920 02	0.37687396700 02

VIRIAL THEOREM
-0.20000214000 01

A-33

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.114093	2.0	0.095838
1.0	0.300728	2.0	0.274838
1.0	0.756743	2.0	0.772812
1.0	2.727595	2.0	2.239237
1.0	6.810816	2.0	7.472611
1.0	17.620929	2.0	32.692074
1.0	46.856223		
1.0	149.433371		
1.0	527.099542		
1.0	2316.472815		
1.0	15469.390094		

S		P	
1.0	0.102590	2.0	0.095840
1.0	0.262970	2.0	0.274840
1.0	0.678100	2.0	0.772810
1.0	2.095880	2.0	2.239240
1.0	4.866880	2.0	7.472610
1.0	11.818100	2.0	32.692100
1.0	30.667400		
1.0	85.779000		
1.0	264.795000		
1.0	939.514000		
1.0	4143.520000		
1.0	27736.600000		

ORBITAL ENERGIES, EIGENVECTORS,

-11.32547	-0.70560	-0.43317
0.001320	-0.302890	0.230901
-0.004412	-0.587849	0.462732
0.020133	-0.253419	0.351470
0.254118	0.135177	0.151011
0.421504	0.139977	0.039121
0.288316	0.070928	0.005869
0.123636	0.028208	0.0
0.039167	0.008465	0.0
0.009743	0.002098	0.0
0.001879	0.000400	0.0
0.000242	0.000052	0.0

-11.32560	-0.70562	-0.43321
0.000292	-0.235649	0.230902
-0.000526	-0.581813	0.462713
0.007176	-0.328896	0.351486
0.146231	0.079219	0.151013
0.377591	0.151697	0.039122
0.349354	0.092481	0.005869
0.182120	0.042990	0.0
0.067683	0.014833	0.0
0.019857	0.004302	0.0
0.004787	0.001019	0.0
0.000912	0.000195	0.0
0.000117	0.000025	0.0

CARBON 11/7 DERIVED SET

TOTAL HF ENERGY
-0.37688203970 02

POTENTIAL ENERGY KINETIC ENERGY
-0.75375789000 02 0.37687585130 02

VIRIAL THEOREM
-0.20000164180 01

CARBOM 12/7 SOURCE SET

TOTAL HF ENERGY
-0.37688386600 02

POTENTIAL ENERGY KINETIC ENERGY
-0.75376125860 02 0.37687739260 02

VIRIAL THEOREM
-0.20000171760 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.114090	2.0	0.077310
1.0	0.300730	2.0	0.198270
1.0	0.756740	2.0	0.505460
1.0	2.727600	2.0	1.324870
1.0	6.810820	2.0	3.772240
1.0	17.620900	2.0	12.339700
1.0	48.856200	2.0	51.723300
1.0	149.438000		
1.0	527.099000		
1.0	2316.470000		
1.0	15469.400000		

S		P	
1.0	0.102594	2.0	0.077314
1.0	0.262973	2.0	0.198268
1.0	0.678103	2.0	0.505457
1.0	2.096878	2.0	1.324869
1.0	4.866884	2.0	3.772243
1.0	11.818056	2.0	12.339664
1.0	30.667350	2.0	51.723308
1.0	85.778961		
1.0	264.795236		
1.0	939.513997		
1.0	4143.516211		
1.0	27736.592059		

ORBITAL ENERGIES,EIGENVECTORS

-11.32541	-0.70560	-0.43327
0.001320	-0.302895	0.139994
-0.004412	-0.587852	0.384100
0.020134	-0.253410	0.388443
0.254121	0.135178	0.227779
0.421501	-0.139974	0.080806
0.288316	0.070927	0.018979
0.123636	0.028208	0.002734
0.039167	0.008465	0.0
0.009743	0.002098	0.0
0.001879	0.000400	0.0
0.000242	0.000052	0.0
0.1000D-05	0.10000-05	0.1000D-05

-11.32555	-0.70563	-0.43331
0.000292	-0.235672	0.140016
-0.000526	-0.581793	0.384051
0.007176	-0.328899	0.388471
0.146235	0.079231	0.227778
0.377588	0.151688	0.080810
0.349353	0.092484	0.018979
0.182120	0.042989	0.002734
0.067684	0.014833	0.0
0.019857	0.004302	0.0
0.004787	0.001019	0.0
0.000912	0.000195	0.0
0.000117	0.000025	0.0

CARBON 13/7 DERIVED SET

TOTAL HF ENERGY
-0.37688469880 02

POTENTIAL ENERGY KINETIC ENERGY
-0.75376552190 02 0.37688082310 02

VIRIAL THEOREM
-0.20000102830 01

CARBON 13/8 SOURCE SET

TOTAL HF ENERGY
-0.37688522170 02

POTENTIAL ENERGY KINETIC ENERGY
-0.75376792560 02 0.37688270400 02

VIRIAL THEOREM
-0.20000066800 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.099090	2.0	0.077310
1.0	0.246070	2.0	0.198270
1.0	0.613010	2.0	0.505460
1.0	1.547120	2.0	1.324870
1.0	3.577020	2.0	3.772240
1.0	8.383980	2.0	12.339700
1.0	20.659300	2.0	51.723300
1.0	53.918700		
1.0	151.711000		
1.0	472.823000		
1.0	1694.330000		
1.0	7524.790000		
1.0	50557.500000		

S		P	
1.0	0.099087	2.0	0.065429
1.0	0.246068	2.0	0.154740
1.0	0.613013	2.0	0.361944
1.0	1.547118	2.0	0.865150
1.0	3.577015	2.0	2.179317
1.0	8.383976	2.0	6.080365
1.0	20.659311	2.0	19.557611
1.0	53.918746	2.0	83.333155
1.0	151.710752		
1.0	472.822789		
1.0	1694.327599		
1.0	7524.785601		
1.0	50557.500670		

ORBITAL ENERGIES,EIGENVECTORS

-11.32556	-0.70564	-0.43330
-0.000039	-0.212384	0.140017
0.000781	-0.554306	0.384060
0.000830	-0.365023	0.388466
0.068527	0.014896	0.227776
0.308220	0.150919	0.080809
0.383929	0.113393	0.018979
0.241255	0.059073	0.002734
0.104185	0.023375	0.0
0.035217	0.007673	0.0
0.009872	0.002113	0.0
0.002316	0.000495	0.0
0.000434	0.000092	0.0
0.000055	0.000012	0.0

-11.32552	-0.70563	-0.43333
-0.000039	-0.212380	0.087208
0.000781	-0.554321	0.304921
0.000830	-0.365014	0.380144
0.068527	0.014898	0.282296
0.308219	0.150917	0.135108
0.383929	0.113392	0.042873
0.241255	0.059073	0.009640
0.104184	0.023375	0.001254
0.035217	0.007673	0.0
0.009872	0.002113	0.0
0.002316	0.000495	0.0
0.000434	0.000092	0.0
0.000055	0.000012	0.0

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0.0	0.0	-0.33333333	-0.13333333	0.0	0.0
0.0	0.0	0.0	0.0	0.0	

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NITROGEN 4/2 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.53862888380 02

POTENTIAL ENERGY -0.10774313110 03 KINETIC ENERGY 0.53880242730 02

VIRIAL THEOREM
-0.19996779090 01

NITROGEN 5/2 SOURCE SET

TOTAL HF ENERGY
-0.54079916120 02

POTENTIAL ENERGY -0.10816040550 03 KINETIC ENERGY 0.54080489360 02

VIRIAL THEOREM
-0.19999894000 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.424895	2.0	0.415430
1.0	6.999433	2.0	2.337950
1.0	32.636131		
1.0	217.231337		

S		P	
1.0	0.424281	2.0	0.415430
1.0	5.666831	2.0	2.337951
1.0	21.226649		
1.0	94.738456		
1.0	628.502795		

ORBITAL ENERGIES,EIGENVECTORS

-15.52850	-0.89871	-0.47868
0.036668	1.038246	0.803396
0.663608	-0.222896	0.341510
0.386545	-0.096806	0.0
0.067831	-0.014486	0.0

-15.64022	-0.90051	-0.48121
0.022854	-1.042364	0.802561
0.532591	0.179465	0.342661
0.448778	0.126246	0.0
0.131732	0.027951	0.0
0.018969	0.004201	0.0

NITROGEN 6/2 DERIVED SET

TOTAL HF ENERGY
-0.54142168540 02

POTENTIAL ENERGY -0.10829167020 03
KINETIC ENERGY 0.54149501660 02

VIRIAL THEOREM
-0.19998645760 01

NITROGEN 5/3 DERIVED SET

TOTAL HF ENERGY
-0.54231284880 02

POTENTIAL ENERGY -0.10848554870 03
KINETIC ENERGY 0.54254263780 02

VIRIAL THEOREM
-0.19995764590 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.259530	2.0	0.415430
1.0	0.839540	2.0	2.337950
1.0	6.106400		
1.0	22.906600		
1.0	102.266000		
1.0	678.719000		

S		P	
1.0	0.424280	2.0	0.291590
1.0	5.666830	2.0	1.261310
1.0	21.226600	2.0	6.127970
1.0	94.738500		
1.0	628.503000		

ORBITAL ENERGIES, EIGENVECTORS

-15.64171	-0.93314	-0.49266
-0.016319	-0.677450	0.802450
0.055723	-0.434523	0.342814
0.547576	0.224379	0.0
0.427207	0.113786	0.0
0.120654	0.027741	0.0
0.017280	0.003866	0.0

-15.59504	-0.90299	-0.53419
0.023289	-1.042510	0.619279
0.533315	0.180502	0.469220
0.447974	0.125870	0.115937
0.131683	0.028020	0.0
0.018952	0.004200	0.0

NITROGEN 6/3 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.5429461057D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.1085899817D 03	0.5429537111D 02

VIRIAL THEOREM
-0.1999985992D 01

NITROGEN 7/3 SOURCE SET

TOTAL HF ENERGY
-0.5433983922D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.1086813630D 03	0.5434152373D 02

VIRIAL THEOREM
-0.1999969002D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.258533	2.0	0.291590
1.0	0.839544	2.0	1.261310
1.0	6.106404	2.0	6.127970
1.0	22.906555		
1.0	102.265549		
1.0	678.718727		

S		P	
1.0	0.237369	2.0	0.291589
1.0	0.780879	2.0	1.261308
1.0	5.133083	2.0	6.127965
1.0	16.718850		
1.0	60.359905		
1.0	266.305188		
1.0	1771.539751		

ORBITAL ENERGIES,EIGENVECTORS

-15.60091	-0.93679	-0.54742
-0.016566	-0.681706	0.618984
0.056596	-0.429649	0.469610
0.547964	0.224216	0.115809
0.426499	0.113289	0.0
0.120603	0.027716	0.0
0.017266	0.003857	0.0

-15.62433	-0.93839	-0.54829
-0.009285	-0.618002	0.618555
0.035282	-0.503490	0.469999
0.447533	0.191716	0.115917
0.458061	0.132124	0.0
0.177266	0.041073	0.0
0.039613	0.008974	0.0
0.005309	0.001164	0.0

NITROGEN 8/3 DERIVED SET

TOTAL HF ENERGY
-0.5435143156D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.10H7023160D 03	0.5435083440D 02

VIRIAL THEOREM
-0.2000011907D 01

NITROGEN 7/4 DERIVED SET

TOTAL HF ENERGY
-0.5437337276D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.1087503728D 03	0.5437700006D 02

VIRIAL THEOREM
-0.1999933294D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.229590	2.0	0.291590
1.0	0.761970	2.0	1.261310
1.0	4.464320	2.0	6.127970
1.0	13.110100		
1.0	41.140300		
1.0	146.245000		
1.0	643.220000		
1.0	4284.800000		

S		P	
1.0	0.237370	2.0	0.218880
1.0	0.780880	2.0	0.798920
1.0	5.133080	2.0	2.923070
1.0	16.718900	2.0	13.573100
1.0	60.359900		
1.0	266.305000		
1.0	1771.540000		

ORBITAL ENERGIES,EIGENVECTORS

-15.63063	-0.93872	-0.54865
-0.005412	-0.594640	0.618375
0.023787	-0.531600	0.470161
0.364274	0.160478	0.115964
0.463347	0.145787	0.0
0.276448	0.053311	0.0
0.066609	0.015414	0.0
0.013577	0.002966	0.0
0.001773	0.000394	0.0

-15.61962	-0.94171	-0.56183
-0.009324	-0.618097	0.463265
0.035418	-0.503440	0.509866
0.447665	0.191975	0.216587
0.457919	0.131993	0.039795
0.177228	0.041084	0.0
0.039607	0.008972	0.0
0.005308	0.001165	0.0

NITROGEN 8/4 SOURCE SET

TOTAL HF ENERGY
-0.54385043120 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.10877105670 03	0.54386013580 02

VIRIAL THEOREM
-0.19999821560 01

NITROGEN 9/4 DERIVED SET

TOTAL HF ENERGY
-0.54388370020 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.10877499650 03	0.54386626490 02

VIRIAL THEOREM
-0.20000320580 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.229593	2.0	0.218883
1.0	0.761970	2.0	0.798916
1.0	4.464323	2.0	2.923067
1.0	13.110075	2.0	13.573142
1.0	41.140323		
1.0	146.244810		
1.0	643.220221		
1.0	4284.794149		

S		P	
1.0	0.222620	2.0	0.218880
1.0	0.739610	2.0	0.798920
1.0	2.579790	2.0	2.923070
1.0	9.346770	2.0	13.573100
1.0	25.874400		
1.0	78.904000		
1.0	277.234000		
1.0	1216.020000		
1.0	8104.070000		

ORBITAL ENERGIES,EIGENVECTORS

-15.62594	-0.94204	-0.56218
-0.005441	-0.594714	0.463063
0.023897	-0.531593	0.509981
0.364441	0.160781	0.216669
0.463208	0.145646	0.039811
0.226396	0.053314	0.0
0.066596	0.015412	0.0
0.013575	0.002966	0.0
0.001773	0.000394	0.0

-15.62763	-0.94228	-0.56243
-0.001889	-0.571897	0.462960
0.012054	-0.556126	0.510048
0.244952	0.105398	0.216704
0.447383	0.164377	0.039815
0.298961	0.073386	0.0
0.115204	0.027514	0.0
0.031234	0.006849	0.0
0.006174	0.001384	0.0
0.000802	0.000175	0.0

NITROGEN 9/5 SOURCE SET

TOTAL HF ENERGY
-0.5439583148D 02

POTENTIAL ENERGY -0.1087907332D 03 KINETIC ENERGY 0.5439490168D 02

VIRIAL THEOREM
-0.2000017094D 01

NITROGEN 10/5 DERIVED SET

TOTAL HF ENERGY
-0.5439728752D 02

POTENTIAL ENERGY -0.1087965499D 03 KINETIC ENERGY 0.5439926193D 02

VIRIAL THEOREM
-0.1999963713D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.222617	2.0	0.175948
1.0	0.739610	2.0	0.560511
1.0	3.579794	2.0	1.750842
1.0	9.346767	2.0	5.991227
1.0	25.074419	2.0	26.866987
1.0	76.904023		
1.0	277.234281		
1.0	1216.021464		
1.0	3104.071631		

S		P	
1.0	0.195060	2.0	0.175950
1.0	0.602530	2.0	0.560510
1.0	1.739200	2.0	1.750840
1.0	5.229600	2.0	5.991230
1.0	14.160700	2.0	26.869000
1.0	40.396900		
1.0	125.447000		
1.0	445.296000		
1.0	1963.120000		
1.0	13119.600000		

ORBITAL ENERGIES, EIGENVECTORS

-15.62720	-0.94339	-0.56567
-0.001891	-0.571781	0.342691
0.012064	-0.556289	0.493796
0.245003	0.105517	0.297420
0.447349	0.164331	0.091156
0.248951	0.073404	0.014478
0.115198	0.027509	0.0
0.031233	0.006851	0.0
0.006174	0.001384	0.0
0.000802	0.000175	0.0

-15.62749	-0.94401	-0.56601
0.001653	-0.462127	0.342639
-0.004758	-0.608835	0.493832
0.061481	-0.057317	0.297426
0.380918	0.184760	0.091152
0.416107	0.119593	0.014478
0.208472	0.051257	0.0
0.069825	0.015814	0.0
0.017665	0.003951	0.0
0.003418	0.000752	0.0
0.000440	0.000097	0.0

NITROGEN 10/6 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.5439903796D 02

POTENTIAL ENERGY -0.10879894440 03 KINETIC ENERGY 0.5439906400 02

VIRIAL THEOREM
-0.1999984036D 01

NITROGEN 11/6 SOURCE SET

TOTAL HF ENERGY
-0.5439990407D 02

POTENTIAL ENERGY -0.10879956740 03 KINETIC ENERGY 0.5439966336D 02

VIRIAL THEOREM
-0.2000044425D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.195063	2.0	0.143890
1.0	0.602525	2.0	0.421670
1.0	1.739195	2.0	1.194580
1.0	5.229601	2.0	3.472640
1.0	14.160743	2.0	11.498500
1.0	40.396925	2.0	49.873400
1.0	125.446890		
1.0	445.296000		
1.0	1963.122460		
1.0	13119.583465		

S		P	
1.0	0.160920	2.0	0.142847
1.0	0.436520	2.0	0.417456
1.0	1.110850	2.0	1.182076
1.0	3.948430	2.0	3.436903
1.0	9.929540	2.0	11.380142
1.0	25.817500	2.0	49.370672
1.0	71.795200		
1.0	219.966000		
1.0	776.383000		
1.0	3413.450000		
1.0	22800.200000		

ORBITAL ENERGIES,EIGENVECTORS

-15.62820	-0.94484	-0.56710
0.001654	-0.461897	0.248453
-0.004761	-0.609078	0.459919
0.061489	-0.057301	0.346741
0.390922	0.184787	0.147314
0.416102	0.119603	0.037371
0.208468	0.051265	0.005435
0.069825	0.015815	0.0
0.017665	0.003952	0.0
0.003418	0.000752	0.0
0.000440	0.000097	0.0

-15.62872	-0.94507	-0.56724
0.001519	-0.310304	0.245113
-0.004917	-0.592760	0.458844
0.024406	-0.244222	0.348918
0.271128	0.141927	0.149026
0.423143	0.143038	0.037915
0.277557	0.070425	0.005525
0.115507	0.027201	0.0
0.036023	0.008047	0.0
0.008908	0.001983	0.0
0.001715	0.000377	0.0
0.000221	0.000049	0.0

NITROGEN 12/6 DERIVED SET

TOTAL HF ENERGY
-0.54400161440 02

POTENTIAL ENERGY KINETIC ENERGY
-0.10880005620 03 0.54399894810 02

VIRIAL THEOREM
-0.20000049010 01

NITROGEN 11/7 DERIVED SET

TOTAL HF ENERGY
-0.54400328420 02

POTENTIAL ENERGY KINETIC ENERGY
-0.10880025860 03 0.54399930190 02

VIRIAL THEOREM
-0.20000073200 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.151530	2.0	0.142850
1.0	0.398720	2.0	0.417460
1.0	1.026430	2.0	1.182080
1.0	3.187100	2.0	3.436900
1.0	7.370600	2.0	11.380100
1.0	17.742100	2.0	49.370700
1.0	45.517100		
1.0	126.210000		
1.0	388.042000		
1.0	1374.920000		
1.0	6061.250000		
1.0	40564.500000		

S		P	
1.0	0.160920	2.0	0.118820
1.0	0.436520	2.0	0.316980
1.0	1.110850	2.0	0.820810
1.0	3.948430	2.0	2.143550
1.0	9.929540	2.0	5.997130
1.0	25.817500	2.0	19.382000
1.0	71.795200	2.0	82.771500
1.0	219.966000		
1.0	776.383000		
1.0	3413.450000		
1.0	22800.200000		

ORBITAL ENERGIES,EIGENVECTORS

-15.62885	-0.94509	-0.56725
0.000575	-0.268484	0.245113
-0.001300	-0.583242	0.458841
0.012035	-0.299014	0.348919
0.175004	0.094818	0.149027
0.384095	0.151385	0.037915
0.331021	0.089759	0.005525
0.167957	0.040835	0.0
0.062159	0.014081	0.0
0.018258	0.004088	0.0
0.004406	0.000971	0.0
0.000839	0.000186	0.0
0.000108	0.000024	0.0

-15.62884	-0.94523	-0.56748
0.001519	-0.310263	0.167249
-0.004918	-0.592790	0.397308
0.024407	-0.244233	0.375536
0.271130	0.141934	0.212116
0.423141	0.143039	0.074625
0.277557	0.070426	0.017447
0.115506	0.027201	0.002259
0.036023	0.008047	0.0
0.008908	0.001983	0.0
0.001715	0.000377	0.0
0.000221	0.000049	0.0

NITROGEN 12/7 SOURCE SET

TOTAL HF ENERGY
-0.54400585540 02

POTENTIAL ENERGY -0.10880074020 03
KINETIC ENERGY 0.54400154650 02

VIRIAL THEOREM
-0.20000079210 01

NITROGEN 13/7 DERIVED SET

TOTAL HF ENERGY
-0.54400685010 02

POTENTIAL ENERGY -0.10880107450 03
KINETIC ENERGY 0.54400389500 02

VIRIAL THEOREM
-0.20000054320 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.151533	2.0	0.118819
1.0	0.398715	2.0	0.316975
1.0	1.026431	2.0	0.820812
1.0	3.187096	2.0	2.143546
1.0	7.370599	2.0	5.997132
1.0	17.742148	2.0	19.381951
1.0	45.517104	2.0	82.771495
1.0	126.210297		
1.0	388.041767		
1.0	1374.918050		
1.0	6061.252552		
1.0	40564.454815		

S		P	
1.0	0.141090	2.0	0.118820
1.0	0.358340	2.0	0.316980
1.0	0.901860	2.0	0.820810
1.0	2.333470	2.0	2.143550
1.0	5.265090	2.0	5.997130
1.0	12.263600	2.0	19.382000
1.0	30.237300	2.0	82.771500
1.0	79.615800		
1.0	225.479000		
1.0	703.777000		
1.0	2512.690000		
1.0	11123.700000		
1.0	74761.700000		

ORBITAL ENERGIES,EIGENVECTORS

-15.62897	-0.94525	-0.56749
0.000576	-0.268649	0.167238
-0.001300	-0.583253	0.397311
0.012035	-0.299044	0.376540
0.175006	0.094833	0.212116
0.384095	0.151383	0.074626
0.331020	0.089763	0.017447
0.167955	0.040835	0.002359
0.062159	0.014081	0.0
0.018258	0.004088	0.0
0.004406	0.000971	0.0
0.000839	0.000186	0.0
0.000108	0.000024	0.0

-15.62902	-0.94527	-0.56750
0.000084	-0.223874	0.167250
0.000537	-0.557905	0.397249
0.003101	-0.355916	0.376542
0.082578	0.023368	0.212116
0.318621	0.153968	0.074626
0.377541	0.114055	0.017447
0.231728	0.058537	0.002359
0.097424	0.022560	0.0
0.032081	0.007224	0.0
0.008906	0.001971	0.0
0.002088	0.000462	0.0
0.000394	0.000087	0.0
0.000050	0.000011	0.0

NITROGEN 13/8 SOURCE SET

TOTAL HF ENERGY
-0.5440078196D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.1088012649D 03	0.5440047506D 02

VIRIAL THEOREM
-0.2000005787D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.141093	2.0	0.094264
1.0	0.359336	2.0	0.232449
1.0	0.901856	2.0	0.557696
1.0	2.333471	2.0	1.350000
1.0	5.265086	2.0	3.405104
1.0	12.263622	2.0	9.394038
1.0	30.237283	2.0	29.837389
1.0	79.615810	2.0	126.666567
1.0	225.478793		
1.0	703.777285		
1.0	2512.685697		
1.0	11123.653813		
1.0	74761.715106		

ORBITAL ENERGIES,EIGENVECTORS

-15.62906	-0.94532	-0.56757
0.000054	-0.223862	0.094498
0.000537	-0.557902	0.314966
0.003101	-0.355933	0.380736
0.042578	0.023873	0.277697
0.318623	0.153968	0.130101
0.377540	0.114056	0.040814
0.231728	0.058537	0.009016
0.097424	0.022560	0.001152
0.032081	0.007224	0.0
0.008906	0.001971	0.0
0.002088	0.000462	0.0
0.000394	0.000087	0.0
0.000050	0.000011	0.0

CHARGE = 8.000000

VECTOR COUPLING COEFFICIENTS K

0.0	0.0	-0.16666667	-0.01666667	0.0	0.0
0.0	0.0	0.0	0.0	0.0	

O(^{3}P)

OXYGEN 4/2 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.73975182740 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.14796293320 03	0.73987750450 02

VIRIAL THEOREM
-0.19998301380 01

OXYGEN 5/2 SOURCE SET

TOTAL HF ENERGY
-0.74259473790 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.14851775830 03	0.74259284500 02

VIRIAL THEOREM
-0.19999890830 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.579735	2.0	0.547380
1.0	9.286970	2.0	3.175230
1.0	43.120125		
1.0	286.817626		

S		P	
1.0	0.578468	2.0	0.547378
1.0	7.516443	2.0	3.175230
1.0	27.991244		
1.0	124.506486		
1.0	825.325176		

ORBITAL ENERGIES,EIGENVECTORS

-20.54443	-1.17255	-0.49727
0.037758	1.039556	0.800494
0.663403	-0.226476	0.350088
0.383946	-0.100143	0.0
0.067414	-0.014763	0.0

-20.68808	-1.17502	-0.50000
0.023696	-1.043431	0.799836
0.531653	0.180359	0.350995
0.448627	0.131343	0.0
0.131499	0.029679	0.0
0.018949	0.004329	0.0

OXYGEN 6/2 DERIVED SET

TOTAL HF ENERGY
-0.74346382720 02

POTENTIAL ENERGY KINETIC ENERGY
-0.14870309740 03 0.74356714660 02

VIRIAL THEOREM
-0.19998610490 01

OXYGEN 5/3 DERIVED SET

TOTAL HF ENERGY
-0.74552916860 02

POTENTIAL ENERGY KINETIC ENERGY
-0.14913617900 03 0.74583262170 02

VIRIAL THEOREM
-0.19999593135D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.349190	2.0	0.547380
1.0	1.147960	2.0	3.175230
1.0	8.130700		
1.0	30.382700		
1.0	135.416000		
1.0	898.725000		

S		P	
1.0	0.578470	2.0	0.374850
1.0	7.516440	2.0	1.684710
1.0	27.991200	2.0	8.142200
1.0	124.506000		
1.0	825.325000		

ORBITAL ENERGIES,EIGENVECTORS

-20.69119	-1.21979	-0.51368
-0.016065	-0.674728	0.799753
0.057100	-0.440599	0.351109
0.548035	0.228450	0.0
0.425916	0.117510	0.0
0.119658	0.028252	0.0
0.017093	0.003937	0.0

-20.62319	-1.18302	-0.58350
0.024213	-1.043610	0.616427
0.532543	0.181609	0.474453
0.447642	0.130892	0.122835
0.131637	0.028761	0.0
0.018929	0.004328	0.0

OXYGEN 6/3 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.74642412370 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.14928500750 03	0.74642595110 02

VIRIAL THEOREM
-0.19999975520 01

OXYGEN 7/3 SOURCE SET

TOTAL HF ENERGY
-0.74701078690 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.14940330150 03	0.74702222790 02

VIRIAL THEOREM
-0.19999846840 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.349190	2.0	0.374850
1.0	1.147961	2.0	1.684710
1.0	8.130696	2.0	8.142200
1.0	30.382708		
1.0	135.416016		
1.0	898.725147		

S		P	
1.0	0.321511	2.0	0.374851
1.0	1.070570	2.0	1.684711
1.0	6.820629	2.0	8.142199
1.0	22.119990		
1.0	79.596537		
1.0	350.639740		
1.0	2331.569509		

ORBITAL ENERGIES, EIGENVECTORS

-20.63140	-1.22925	-0.59916
-0.016355	-0.678813	0.616207
0.058145	-0.435938	0.474760
0.548510	0.228500	0.122669
0.425051	0.116962	0.0
0.119593	0.028242	0.0
0.017075	0.003928	0.0

-20.66114	-1.23133	-0.60007
-0.009053	-0.617887	0.615882
0.036316	-0.506969	0.475048
0.447265	0.194238	0.122758
0.457462	0.136917	0.0
0.176707	0.042135	0.0
0.039441	0.009209	0.0
0.005288	0.001193	0.0

OXYGEN 8/3 DERIVED SET

TOTAL HF ENERGY
-0.74716217120 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.14943097770 03	0.74714760570 02

VIRIAL THEOREM
-0.20000194950 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.310480	2.0	0.374850
1.0	1.039830	2.0	1.684710
1.0	5.870770	2.0	8.142200
1.0	17.011700		
1.0	52.896400		
1.0	187.284000		
1.0	821.752000		
1.0	5469.630000		

ORBITAL ENERGIES, EIGENVECTORS

-20.66900	-1.23178	-0.60040
-0.005152	-0.592463	0.615751
0.024201	-0.536659	0.475165
0.357200	0.158241	0.122795
0.462675	0.152267	0.0
0.230832	0.056117	0.0
0.068431	0.016338	0.0
0.014016	0.003151	0.0
0.001834	0.000420	0.0

OXYGEN 7/4 DERIVED SET

TOTAL HF ENERGY
-0.74766555060 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.14953766850 03	0.74771113390 02

VIRIAL THEOREM
-0.19999390360 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.321510	2.0	0.276060
1.0	1.070570	2.0	1.048560
1.0	6.820620	2.0	3.863290
1.0	22.120000	2.0	17.739400
1.0	79.596500		
1.0	350.640000		
1.0	2331.570000		

ORBITAL ENERGIES, EIGENVECTORS

-20.65551	-1.23799	-0.62232
-0.009100	-0.617706	0.461676
0.036479	-0.507250	0.508157
0.447426	0.194620	0.228295
0.457288	0.136777	0.042861
0.176658	0.042158	0.0
0.039433	0.009208	0.0
0.005287	0.001193	0.0

OXYGEN 8/4 SOURCE SET

TOTAL HF ENERGY
-0.74781739950 02

POTENTIAL ENERGY KINETIC ENERGY
-0.14956486440 03 0.74783124430 02

VIRIAL THEOREM
-0.19999814870 01

OXYGEN 9/4 DERIVED SET

TOTAL HF ENERGY
-0.74786147690 02

POTENTIAL ENERGY KINETIC ENERGY
-0.14957204200 03 0.74785894300 02

VIRIAL THEOREM
-0.20000033880 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.310478	2.0	0.276060
1.0	1.039829	2.0	1.048558
1.0	5.870769	2.0	3.863290
1.0	17.011654	2.0	17.739374
1.0	52.896390		
1.0	187.284146		
1.0	821.752352		
1.0	5469.626707		

S		P	
1.0	0.300690	2.0	0.276060
1.0	1.004270	2.0	1.048560
1.0	4.756800	2.0	3.863290
1.0	12.287500	2.0	17.739400
1.0	33.905800		
1.0	103.652000		
1.0	364.725000		
1.0	1599.710000		
1.0	10662.300000		

ORBITAL ENERGIES, EIGENVECTORS

-20.66338	-1.23845	-0.62265
-0.005185	-0.592232	0.461533
0.024329	-0.537025	0.508236
0.357408	0.158682	0.228355
0.462507	0.152117	0.042873
0.230764	0.056130	0.0
0.068414	0.016338	0.0
0.014013	0.003151	0.0
0.001834	0.000420	0.0

-20.66544	-1.23878	-0.62288
-0.001984	-0.567745	0.461466
0.013165	-0.561584	0.509277
0.243110	0.101956	0.228379
0.444910	0.170145	0.042876
0.301564	0.076600	0.0
0.115603	0.028464	0.0
0.031158	0.007035	0.0
0.006153	0.001420	0.0
0.000800	0.000180	0.0

OXYGEN 9/5 SOURCE SET

TOTAL HF ENERGY
-0.74800948980 02

POTENTIAL ENERGY -0.14960084290 03
KINETIC ENERGY 0.74799893910 02

VIRIAL THEOREM
-0.20000141050 01

OXYGEN 10/5 DERIVED SET

TOTAL HF ENERGY
-0.74903039180 02

POTENTIAL ENERGY -0.14960791480 03
KINETIC ENERGY 0.74804875580 02

VIRIAL THEOREM
-0.19999754510 01

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BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.300686	2.0	0.214882
1.0	1.004271	2.0	0.723164
1.0	4.756803	2.0	2.308269
1.0	12.287469	2.0	7.843131
1.0	33.905805	2.0	34.856463
1.0	103.651793		
1.0	364.725257		
1.0	1599.709689		
1.0	10662.284940		

S		P	
1.0	0.252910	2.0	0.214880
1.0	0.760670	2.0	0.723160
1.0	2.018420	2.0	2.308270
1.0	6.628090	2.0	7.843130
1.0	17.989200	2.0	34.856500
1.0	51.284000		
1.0	159.262000		
1.0	565.236000		
1.0	2488.820000		
1.0	16619.900000		

ORBITAL ENERGIES, EIGENVECTORS

-20.66643	-1.24182	-0.62905
-0.001986	-0.567341	0.339516
0.013176	-0.562082	0.492470
0.243172	0.102146	0.307748
0.444870	0.170109	0.098197
0.301552	0.076637	0.015648
0.115596	0.028463	0.0
0.031157	0.007038	0.0
0.006153	0.001420	0.0
0.000799	0.000180	0.0

-20.66693	-1.24277	-0.62954
0.002234	-0.425442	0.339470
-0.007308	-0.609010	0.492494
0.053175	-0.103241	0.307766
0.371664	0.184245	0.098193
0.424078	0.129334	0.015648
0.216035	0.054655	0.0
0.072588	0.017045	0.0
0.018391	0.004222	0.0
0.003563	0.000810	0.0
0.000460	0.000104	0.0

OXYGEN 10/6 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.74806538809D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.14961509960 03	0.74808561460 02

VIRIAL THEOREM
-0.19999729530 01

OXYGEN 11/6 SOURCE SET

TOTAL HF ENERGY
-0.74807620370 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.14961595770 03	0.74808337350 02

VIRIAL THEOREM
-0.19999904160 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.252912	2.0	0.177760
1.0	0.760669	2.0	0.541070
1.0	2.018416	2.0	1.563690
1.0	6.628092	2.0	4.554400
1.0	17.989164	2.0	14.972700
1.0	51.284014	2.0	64.771900
1.0	159.262017		
1.0	565.235767		
1.0	2488.824590		
1.0	16619.901297		

S		P	
1.0	0.220544	2.0	0.177759
1.0	0.605501	2.0	0.541065
1.0	1.538729	2.0	1.563689
1.0	5.386177	2.0	4.554398
1.0	13.617874	2.0	14.972658
1.0	35.460926	2.0	64.771949
1.0	98.515283		
1.0	301.425731		
1.0	1062.617249		
1.0	4669.379711		
1.0	31195.564766		

ORBITAL ENERGIES,EIGENVECTORS

-20.66724	-1.24354	-0.63103
0.002235	-0.425313	0.251392
-0.007312	-0.609154	0.450345
0.053187	-0.103219	0.352982
0.371668	0.184265	0.157534
0.424072	0.129334	0.040573
0.216031	0.054660	0.005844
0.072587	0.017045	0.0
0.018390	0.004222	0.0
0.003563	0.000810	0.0
0.000460	0.000104	0.0

-20.66787	-1.24373	-0.63115
0.001640	-0.320019	0.251382
-0.005144	-0.591220	0.450332
0.027483	-0.238690	0.353003
0.283034	0.147889	0.157536
0.423548	0.146007	0.040575
0.269493	0.070296	0.005844
0.110311	0.026718	0.0
0.034191	0.007860	0.0
0.008450	0.001936	0.0
0.001628	0.000369	0.0
0.000210	0.000048	0.0

OXYGEN 12/6 DERIVED SET

TOTAL HF ENERGY
-0.7480796258D 02

POTENTIAL ENERGY -0.1496162592D 03 KINETIC ENERGY 0.7480829666D 02

VIRIAL THEOREM
-0.1999995534D 01

OXYGEN 11/7 DERIVED SET

TOTAL HF ENERGY
-0.7480849135D 02

POTENTIAL ENERGY -0.1496172983D 03 KINETIC ENERGY 0.7480880699D 02

VIRIAL THEOREM
-0.1999995781D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.206190	2.0	0.177760
1.0	0.548530	2.0	0.541070
1.0	1.408210	2.0	1.563690
1.0	4.383550	2.0	4.554400
1.0	10.217500	2.0	14.972700
1.0	24.614300	2.0	64.771900
1.0	63.321200		
1.0	176.046000		
1.0	542.474000		
1.0	1929.080000		
1.0	6526.180000		
1.0	57134.200000		

S		P	
1.0	0.220540	2.0	0.150740
1.0	0.605500	2.0	0.423600
1.0	1.538730	2.0	1.128480
1.0	5.386180	2.0	2.972370
1.0	13.617900	2.0	8.320770
1.0	35.460900	2.0	26.876700
1.0	98.515300	2.0	114.863000
1.0	301.426000		
1.0	1062.620000		
1.0	4669.380000		
1.0	31195.600000		

ORBITAL ENERGIES, EIGENVECTORS.

-20.66808	-1.24377	-0.63119
0.000644	-0.274508	0.251384
-0.001337	-0.580697	0.450323
0.013896	-0.298260	0.353007
0.189678	0.101202	0.157537
0.389233	0.154856	0.040576
0.322623	0.089511	0.005844
0.160040	0.039999	0.0
0.058126	0.013531	0.0
0.016952	0.003908	0.0
0.004064	0.000921	0.0
0.000770	0.000175	0.0
0.000099	0.000022	0.0

-20.66817	-1.24407	-0.63163
0.001640	-0.319941	0.184703
-0.005144	-0.591286	0.398523
0.027484	-0.238701	0.370478
0.293038	0.147898	0.212775
0.423545	0.146011	0.075341
0.269493	0.070298	0.017192
0.110311	0.026719	0.002266
0.034191	0.007860	0.0
0.008450	0.001936	0.0
0.001628	0.000369	0.0
0.000210	0.000048	0.0

OXYGEN 12/7 SOURCE SET

TOTAL HF ENERGY
-0.74808833080 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.14961759180 03	0.74808758750 02

VIRIAL THEOREM
-0.20000009940 01

OXYGEN 13/7 DERIVED SET

TOTAL HF ENERGY
-0.74808962930 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.14961798270 03	0.74809019800 02

VIRIAL THEOREM
-0.19999992400 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.206187	2.0	0.150740
1.0	0.548532	2.0	0.423603
1.0	1.408205	2.0	1.128482
1.0	4.383550	2.0	2.972366
1.0	10.217494	2.0	8.320766
1.0	24.614264	2.0	26.876666
1.0	63.321180	2.0	114.863473
1.0	176.045943		
1.0	542.473877		
1.0	1929.082677		
1.0	8526.182827		
1.0	57134.233349		

S		P	
1.0	0.191670	2.0	0.150740
1.0	0.495160	2.0	0.423600
1.0	1.253880	2.0	1.128480
1.0	3.222860	2.0	2.972370
1.0	7.438310	2.0	8.320770
1.0	17.395600	2.0	26.876700
1.0	42.699500	2.0	114.863000
1.0	111.654000		
1.0	315.979000		
1.0	987.365000		
1.0	3534.540000		
1.0	15679.200000		
1.0	105375.000000		

ORBITAL ENERGIES,EIGENVECTORS

-20.66838	-1.24411	-0.63167
0.000644	-0.274438	0.184710
-0.001338	-0.580745	0.398510
0.013896	-0.298285	0.370484
0.189681	0.101215	0.212776
0.389230	0.154857	0.075343
0.322624	0.089516	0.017192
0.160039	0.040000	0.002266
0.058127	0.013531	0.0
0.016952	0.003908	0.0
0.004064	0.000921	0.0
0.000770	0.000175	0.0
0.000099	0.000022	0.0

-20.66845	-1.24414	-0.63170
-0.000031	-0.230372	0.184715
0.001198	-0.560245	0.398498
0.002669	-0.353405	0.370494
0.096808	0.034398	0.212774
0.337276	0.159936	0.075343
0.368721	0.112807	0.017192
0.217401	0.056288	0.002266
0.090452	0.021512	0.0
0.029725	0.006888	0.0
0.008206	0.001869	0.0
0.001920	0.000437	0.0
0.000361	0.000082	0.0
0.000046	0.000010	0.0

OXYGEN 13/8 SOURCE SET

TOTAL HF ENERGY
-0.74809191590 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.14961829710 03	0.74809105470 02

VIRIAL THEOREM
-0.20000011510 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.191665	2.0	0.128892
1.0	0.495155	2.0	0.337597
1.0	1.253877	2.0	0.850223
1.0	3.222862	2.0	2.102525
1.0	7.438309	2.0	5.313064
1.0	17.395596	2.0	14.621809
1.0	42.699451	2.0	46.533367
1.0	111.654281	2.0	200.000000
1.0	315.978752		
1.0	987.365160		
1.0	3534.544676		
1.0	15679.240331		
1.0	105374.945317		

ORBITAL ENERGIES, EIGENVECTORS

-20.66856	-1.24425	-0.63184
-0.000031	-0.230347	0.130297
0.001198	-0.560252	0.344042
0.002669	-0.353426	0.374236
0.096808	0.034404	0.255983
0.337277	0.159936	0.114877
0.368720	0.112808	0.034863
0.217402	0.056289	0.007351
0.090452	0.021513	0.000892
0.029725	0.006888	0.0
0.008206	0.001869	0.0
0.001920	0.000437	0.0
0.000361	0.000082	0.0
0.000046	0.000010	0.0

$F(^2P)$

CHARGE = 9.000000

VECTOR COUPLING COEFFICIENTS K

0.0	0.0	-0.06666667	0.00533333	0.0	0.0
0.0	0.0	0.0	0.0	0.0	

FLUORINE 4/2 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.98181755510 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.19638418450 03	0.98202429010 02

VIRIAL THEOREM
-0.19997894810 01

FLUORINE 5/2 SOURCE SET

TOTAL HF ENERGY
-0.98540462010 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.19708285700 03	0.98542395040 02

VIRIAL THEOREM
-0.19999803840 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.755976	2.0	0.709610
1.0	11.901915	2.0	4.175660
1.0	55.068569		
1.0	365.993159		

S		P	
1.0	0.753662	2.0	0.709609
1.0	9.615831	2.0	4.175663
1.0	35.661781		
1.0	158.333486		
1.0	1049.414716		

ORBITAL ENERGIES,EIGENVECTORS

-26.22978	-1.47039	-0.54191
0.038674	1.040355	0.798690
0.663366	-0.228746	0.354750
0.383313	-0.102494	0.0
0.067102	-0.014950	0.0

-26.41045	-1.47368	-0.54503
0.024293	-1.044041	0.798130
0.530591	0.180414	0.355521
0.448894	0.135173	0.0
0.131733	0.029700	0.0
0.018923	0.004418	0.0

FLUORINE 6/2 DERIVED SET

TOTAL HF ENERGY
-0.99658079330 02

POTENTIAL ENERGY KINETIC ENERGY
-0.19733258540 03 0.98674506030 02

VIRIAL THEOREM
-0.19998335260 01

FLUORINE 5/3 DERIVED SET

TOTAL HF ENERGY
-0.99041086660 02

POTENTIAL ENERGY KINETIC ENERGY
-0.19812089920 03 0.99079812510 02

VIRIAL THEOREM
-0.19996091450 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.453740	2.0	0.709610
1.0	1.506680	2.0	4.175660
1.0	10.447700		
1.0	38.960600		
1.0	173.564000		
1.0	1152.220000		

S		P	
1.0	0.753660	2.0	0.478820
1.0	9.615830	2.0	2.192980
1.0	35.661300	2.0	10.559800
1.0	158.333000		
1.0	1049.410000		

ORBITAL ENERGIES,EIGENVECTORS

-26.41544	-1.53223	-0.56082
-0.015857	-0.676219	0.798065
0.058314	-0.441304	0.355609
0.548696	0.231284	0.0
0.424790	0.120059	0.0
0.118656	0.028533	0.0
0.016900	0.003971	0.0

-26.32355	-1.48887	-0.66418
0.024869	-1.044248	0.614012
0.531617	0.181834	0.477755
0.447765	0.134658	0.126663
0.131659	0.029291	0.0
0.018901	0.004416	0.0

FLUORINE 6/3 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.9916102776D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.19832361190 03	0.99162584130 02

VIRIAL THEOREM
-0.19999843050 01

FLUORINE 7/3 SOURCE SET

TOTAL HF ENERGY
-0.99234933140 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.19847006990 03	0.99235136710 02

VIRIAL THEOREM
-0.19999979490 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.453735	2.0	0.478820
1.0	1.506684	2.0	2.192980
1.0	10.447704	2.0	10.559800
1.0	38.960593		
1.0	173.564075		
1.0	1152.216979		

S		P	
1.0	0.416741	2.0	0.478821
1.0	1.401691	2.0	2.192976
1.0	8.731837	2.0	10.559831
1.0	28.233599		
1.0	101.393591		
1.0	446.334663		
1.0	2967.439525		

ORBITAL ENERGIES,EIGENVECTORS

-26.33432	-1.54924	-0.68218
-0.016178	-0.680142	0.613836
0.059491	-0.436838	0.478013
0.545237	0.231507	0.126504
0.423801	0.119470	0.0
0.118580	0.028536	0.0
0.016880	0.003963	0.0

-26.37137	-1.55149	-0.68326
-0.008812	-0.618175	0.613556
0.036944	-0.509101	0.478259
0.446446	0.195474	0.126553
0.457491	0.140543	0.0
0.176507	0.042928	0.0
0.039337	0.009377	0.0
0.005274	0.001213	0.0

FLUORINE 8/3 DERIVED SET

TOTAL HF ENERGY
-0.99254055110 02

POTENTIAL ENERGY KINETIC ENERGY
-0.19850769550 03 0.99253640350 02

VIRIAL THEOREM
-0.20000041790 01

FLUORINE 7/4 DERIVED SET

TOTAL HF ENERGY
-0.99346202910 02

POTENTIAL ENERGY KINETIC ENERGY
-0.19869715470 03 0.99350951830 02

VIRIAL THEOREM
-0.19999522010 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.401210	2.0	0.478820
1.0	1.357000	2.0	2.192980
1.0	7.603850	2.0	10.559800
1.0	22.221800		
1.0	69.402300		
1.0	246.236000		
1.0	1092.680000		
1.0	7213.140000		

S		P	
1.0	0.416740	2.0	0.348120
1.0	1.401690	2.0	1.351190
1.0	8.731840	2.0	4.993480
1.0	28.233600	2.0	22.747600
1.0	101.394000		
1.0	446.335000		
1.0	2967.440000		

ORBITAL ENERGIES, EIGENVECTORS

-26.38119	-1.55261	-0.68368
-0.005191	-0.591064	0.613441
0.025373	-0.540026	0.478360
0.364628	0.161456	0.126615
0.462607	0.154996	0.0
0.225306	0.055757	0.0
0.065903	0.016054	0.0
0.013414	0.003072	0.0
0.001750	0.000409	0.0

-26.36533	-1.56300	-0.71593
-0.008864	-0.617749	0.459390
0.037127	-0.509676	0.508071
0.446651	0.195957	0.234940
0.457294	0.140403	0.044648
0.176450	0.042960	0.0
0.039327	0.009377	0.0
0.005273	0.001213	0.0

FLUORINE 8/4 SOURCE SET

TOTAL HF ENERGY
-0.99365399610 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.19873412970 03	0.99368730C90 02

VIRIAL THEOREM
-0.19999664840 01

FLUORINE 9/4 DERIVED SET

TOTAL HF ENERGY
-0.99371041140 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.19874321940 03	0.99372178220 02

VIRIAL THEOREM
-0.19999885570 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.401207	2.0	0.348122
1.0	1.356999	2.0	1.351188
1.0	7.608848	2.0	4.993482
1.0	22.721846	2.0	22.747628
1.0	69.402273		
1.0	246.236300		
1.0	1082.676438		
1.0	7213.137989		

S		P	
1.0	0.388870	2.0	0.348120
1.0	1.307220	2.0	1.351190
1.0	6.032230	2.0	4.993480
1.0	15.571400	2.0	22.747600
1.0	42.974500		
1.0	131.374000		
1.0	442.374000		
1.0	2028.690000		
1.0	13521.500000		

ORBITAL ENERGIES,EIGENVECTORS

-26.37516	-1.56364	-0.71635
-0.005229	-0.590572	0.459268
0.025518	-0.540703	0.508137
0.364865	0.161998	0.234993
0.462415	0.154847	0.044659
0.225229	0.055782	0.0
0.065885	0.016057	0.0
0.013411	0.003074	0.0
0.001750	0.000409	0.0

-26.37749	-1.56409	-0.71651
-0.001758	-0.565553	0.459230
0.013119	-0.565059	0.508161
0.239043	0.098169	0.235005
0.445947	0.175297	0.044659
0.303605	0.079054	0.0
0.116089	0.029190	0.0
0.031246	0.007201	0.0
0.006164	0.001451	0.0
0.000801	0.000184	0.0

FLUORINE 9/5 SOURCE SET

TOTAL HF ENERGY
-0.9939635144D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.1987915011D 03	0.9939514967D 02

VIRIAL THEOREM
-0.2000012091D 01

FLUORINE 10/5 DERIVED SET

TOTAL HF ENERGY
-0.9939905146D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.1987995586D 03	0.9940050717D 02

VIRIAL THEOREM
-0.1999985355D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.389869	2.0	0.266824
1.0	1.307215	2.0	0.918597
1.0	6.032232	2.0	2.953246
1.0	15.571440	2.0	9.993426
1.0	42.974531	2.0	44.147303
1.0	131.373661		
1.0	462.373920		
1.0	2028.691629		
1.0	13521.522627		

S		P	
1.0	0.333180	2.0	0.266820
1.0	1.039890	2.0	0.918600
1.0	2.933750	2.0	2.953250
1.0	8.964970	2.0	9.993430
1.0	24.434900	2.0	44.147300
1.0	70.048400		
1.0	217.364000		
1.0	767.434000		
1.0	3366.140000		
1.0	22451.900000		

ORBITAL ENERGIES, EIGENVECTORS

-26.37976	-1.56908	-0.72595
-0.001761	-0.565009	0.335899
0.013129	-0.565720	0.489353
0.239115	0.098401	0.315418
0.445904	0.175263	0.103481
0.303589	0.079100	0.016509
0.116081	0.029190	0.0
0.031244	0.007205	0.0
0.006164	0.001451	0.0
0.000801	0.000184	0.0

-26.38065	-1.57027	-0.72663
0.001882	-0.443968	0.335857
-0.005092	-0.617134	0.489367
0.063498	-0.074623	0.315442
0.387149	0.191633	0.103480
0.416682	0.127128	0.016509
0.203183	0.052383	0.0
0.066716	0.015909	0.0
0.016886	0.003961	0.0
0.003290	0.000761	0.0
0.000425	0.000099	0.0

FLUORINE 10/6 DERIVED SOURCE SET

TOTAL HF ENERGY
-0.99405086620 02

POTENTIAL ENERGY KINETIC ENERGY
-0.19881266630 03 0.99407579680 02

VIRIAL THEOREM
-0.19999749210 01

FLUORINE 11/6 SOURCE SET

TOTAL HF ENERGY
-0.99406533810 02

POTENTIAL ENERGY KINETIC ENERGY
-0.19881382780 03 0.99407299970 02

VIRIAL THEOREM
-0.19999923530 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.333183	2.0	0.219430
1.0	1.039890	2.0	0.678730
1.0	2.933753	2.0	1.976580
1.0	8.964972	2.0	5.771650
1.0	24.434934	2.0	18.934800
1.0	70.048413	2.0	81.849600
1.0	217.363706		
1.0	767.434000		
1.0	3366.143898		
1.0	22451.911474		

S		P	
1.0	0.280332	2.0	0.219427
1.0	0.773155	2.0	0.678728
1.0	1.985517	2.0	1.976580
1.0	6.838301	2.0	5.771647
1.0	17.235234	2.0	18.934810
1.0	44.767419	2.0	81.849627
1.0	124.177566		
1.0	379.579360		
1.0	1338.036521		
1.0	5882.855263		
1.0	39319.330179		

ORBITAL ENERGIES,EIGENVECTORS

-26.36098	-1.57132	-0.72875
0.001883	-0.443846	0.247768
-0.005095	-0.617279	0.442433
0.063510	-0.076588	0.359734
0.387154	0.191651	0.166505
0.416673	0.127126	0.043286
0.203179	0.052388	0.006169
0.066716	0.015909	0.0
0.016886	0.003961	0.0
0.003290	0.000741	0.0
0.000425	0.000099	0.0

-26.38163	-1.57161	-0.72884
0.001535	-0.309639	0.247757
-0.004527	-0.592359	0.442438
0.027026	-0.251066	0.359737
0.279005	0.146369	0.166508
0.423730	0.150437	0.043288
0.271581	0.072569	0.006169
0.111313	0.027557	0.0
0.034537	0.008102	0.0
0.008542	0.001997	0.0
0.001644	0.000380	0.0
0.000212	0.000049	0.0

FLUORINE 12/6 DERIVED SET

TOTAL HF ENERGY
-0.9940693537D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.1988140433D 03	0.9940710797D 02

VIRIAL THEOREM
-0.1999998264D 01

FLUORINE 11/7 DERIVED SET

TOTAL HF ENERGY
-0.9940804383D 02

POTENTIAL ENERGY	KINETIC ENERGY
-0.1988157684D 03	0.9940772452D 02

VIRIAL THEOREM
-0.2000003212D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.255390	2.0	0.219430
1.0	0.676470	2.0	0.678730
1.0	1.742730	2.0	1.976580
1.0	5.018040	2.0	5.771650
1.0	11.553200	2.0	18.934800
1.0	27.581600	2.0	81.849600
1.0	70.212100		
1.0	193.606000		
1.0	592.710000		
1.0	2095.830000		
1.0	9235.450000		
1.0	61799.200000		

S		P	
1.0	0.280330	2.0	0.174860
1.0	0.773160	2.0	0.505550
1.0	1.985520	2.0	1.359510
1.0	6.838300	2.0	3.600210
1.0	17.235200	2.0	10.019300
1.0	44.767400	2.0	32.073400
1.0	124.178000	2.0	136.521000
1.0	379.579000		
1.0	1338.040000		
1.0	5882.860000		
1.0	39319.300000		

ORBITAL ENERGIES,EIGENVECTORS

-26.38187	-1.57168	-0.72889
0.000317	-0.250237	0.247760
0.000055	-0.572924	0.442425
0.009129	-0.330431	0.359745
0.150006	0.074123	0.166508
0.374523	0.162614	0.043288
0.345040	0.101329	0.006169
0.181087	0.046763	0.0
0.068149	0.016297	0.0
0.020247	0.004766	0.0
0.004916	0.001138	0.0
0.000938	0.000218	0.0
0.000120	0.000028	0.0

-26.38225	-1.57225	-0.72967
0.001535	-0.309536	0.270334
-0.004527	-0.592444	0.382700
0.027027	-0.251086	0.373512
0.279008	0.146381	0.229995
0.423727	0.150444	0.095070
0.271582	0.072573	0.019413
0.111312	0.027559	0.002641
0.034537	0.008102	0.0
0.008542	0.001998	0.0
0.001644	0.000390	0.0
0.000212	0.000049	0.0

FLUORINE 12/7 SOURCE SET

TOTAL HF ENERGY
-0.99408444220 02

POTENTIAL ENERGY -0.19881595800 03 KINETIC ENERGY 0.99407514500 02

VIRIAL THEOREM
-0.20000093520 01

FLUORINE 13/7 DERIVED SET

TOTAL HF ENERGY
-0.9940962400D 02

POTENTIAL ENERGY -0.1988166909D 03 KINETIC ENERGY 0.9940805694D 02

VIRIAL THEOREM
-0.2000005704D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.253305	2.0	0.178060
1.0	0.676471	2.0	0.505551
1.0	1.742776	2.0	1.359508
1.0	5.018043	2.0	3.600215
1.0	11.553220	2.0	10.018277
1.0	27.581577	2.0	32.073403
1.0	70.212055	2.0	136.521089
1.0	193.605577		
1.0	592.709682		
1.0	2095.931497		
1.0	9215.454491		
1.0	61799.176538		

S		P	
1.0	0.240860	2.0	0.178660
1.0	0.623290	2.0	0.505550
1.0	1.568160	2.0	1.359510
1.0	3.919400	2.0	3.600210
1.0	8.532740	2.0	10.018300
1.0	18.942900	2.0	32.073400
1.0	44.644700	2.0	136.521000
1.0	113.442000		
1.0	314.035000		
1.0	967.095000		
1.0	3441.540000		
1.0	15281.000000		
1.0	103109.000000		

ORBITAL ENERGIES, EIGENVECTORS

-26.38240	-1.57232	-0.72973
0.000317	-0.250139	0.170348
0.000055	-0.572979	0.382677
0.009128	-0.330480	0.378524
0.150011	0.074143	0.229994
0.374521	0.162615	0.085072
0.345040	0.101337	0.019813
0.181086	0.046764	0.002642
0.063149	0.016298	0.0
0.020247	0.004766	0.0
0.004916	0.001138	0.0
0.000838	0.000218	0.0
0.000120	0.000028	0.0

-26.38258	-1.57235	-0.72975
0.000099	-0.216803	0.170350
0.000828	-0.552150	0.382674
0.003566	-0.367330	0.378526
0.078164	0.009611	0.229994
0.290864	0.150494	0.085072
0.348004	0.122109	0.019813
0.247198	0.067160	0.002642
0.112264	0.027648	0.0
0.039097	0.009282	0.0
0.011200	0.002609	0.0
0.002668	0.000619	0.0
0.000503	0.000116	0.0
0.000064	0.000015	0.0

FLUORINE 13/8 SOURCE SET

TOTAL HF ENERGY
-0.99409011430 02

POTENTIAL ENERGY KINETIC ENERGY
-0.19881761350 03 0.99408602100 02

VIRIAL THEOREM
-0.20000041180 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.240861	2.0	0.154810
1.0	0.623290	2.0	0.403973
1.0	1.568157	2.0	0.995060
1.0	3.919401	2.0	2.447030
1.0	8.532743	2.0	6.274995
1.0	16.942874	2.0	17.604568
1.0	44.644727	2.0	56.919005
1.0	113.442296	2.0	245.330287
1.0	314.035338		
1.0	967.094830		
1.0	3441.539198		
1.0	15281.006720		
1.0	103109.464234		

ORBITAL ENERGIES,EIGENVECTORS

-26.38265	-1.57246	-0.72993
0.000099	-0.216787	0.123475
0.000928	-0.552157	0.318701
0.003566	-0.367339	0.364928
0.078165	0.009616	0.278867
0.290864	0.150493	0.134425
0.368004	0.122110	0.040611
0.247199	0.067160	0.008257
0.112263	0.027648	0.000985
0.039097	0.009282	0.0
0.011200	0.002609	0.0
0.002668	0.000619	0.0
0.000503	0.000116	0.0
0.000064	0.000015	0.0

CHARGE = 10.000000

VECTOR COUPLING COEFFICIENTS K

0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	

Ne(^{1}S)

NEON 4/2 SOURCE SET

TOTAL HF ENERGY
-0.12681594160 03

POTENTIAL ENERGY KINETIC ENERGY
-0.25365510590 03 0.12683916430 03

VIRIAL THEOREM
-0.19998169130 01

NEON 5/2 SOURCE SET

TOTAL HF ENERGY
-0.12725919790 03

POTENTIAL ENERGY KINETIC ENERGY
-0.25451911150 03 0.12725991360 03

VIRIAL THEOREM
-0.19999943760 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.953523	2.0	0.898920
1.0	14.826671	2.0	5.328700
1.0	68.395175		
1.0	454.176070		

S		P	
1.0	0.969902	2.0	0.898919
1.0	11.959466	2.0	5.328713
1.0	44.200647		
1.0	195.933186		
1.0	1298.350011		

ORBITAL ENERGIES,EIGENVECTORS

-32.58705	-1.79298	-0.60165
0.039323	1.040899	0.797413
0.663006	-0.230126	0.357629
0.383127	-0.104361	0.0
0.066955	-0.015104	0.0

-32.80904	-1.79729	-0.60520
0.024703	-1.044401	0.796926
0.529272	0.179962	0.358298
0.449433	0.138239	0.0
0.131958	0.029628	0.0
0.018938	0.004491	0.0

NEON 6/2 DERIVED SET

TOTAL HF ENERGY
-0.1274105205D 03

POTENTIAL ENERGY	KINETIC ENERGY
-0.2548466551D 03	0.1274361345D 03

VIRIAL THEOREM
-0.1999799005D 01

NEON 5/3 DERIVED SET

TOTAL HF ENERGY
-0.1280393194D 03

POTENTIAL ENERGY	KINETIC ENERGY
-0.2561220499D 03	0.1280827305D 03

VIRIAL THEOREM
-0.1999661070D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.568810	2.0	0.898920
1.0	1.906210	2.0	5.328700
1.0	13.055200		
1.0	48.584000		
1.0	216.174000		
1.0	1434.930000		

S		P	
1.0	0.949900	2.0	0.600310
1.0	11.959500	2.0	2.777120
1.0	44.200600	2.0	13.332900
1.0	195.933000		
1.0	1298.350000		

ORBITAL ENERGIES, EIGENVECTORS

-32.81625	-1.87144	-0.62318
-0.015751	-0.675635	0.796870
0.059327	-0.443639	0.358375
0.549251	0.233127	0.0
0.423742	0.121918	0.0
0.117976	0.028747	0.0
0.016780	0.004001	0.0

-32.69796	-1.82131	-0.76510
0.025324	-1.044632	0.611700
0.530409	0.181520	0.480248
0.448188	0.137671	0.129193
0.131813	0.029726	0.0
0.018912	0.004489	0.0

NEON 6/3 SOURCE SET

TOTAL HF ENERGY
-0.12819400150 03

POTENTIAL ENERGY KINETIC ENERGY
-0.25639126160 03 0.12819726020 03

VIRIAL THEOREM
-0.19999745800 01

NEON 7/3 SOURCE SET

TOTAL HF ENERGY
-0.12828494170 03

POTENTIAL ENERGY KINETIC ENERGY
-0.25657270370 03 0.12828776200 03

VIRIAL THEOREM
-0.19999780160 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.568811	2.0	0.600310
1.0	1.906214	2.0	2.777120
1.0	13.055184	2.0	13.332900
1.0	48.584000		
1.0	216.174003		
1.0	1434.926333		

S		P	
1.0	0.523733	2.0	0.600311
1.0	1.775054	2.0	2.777119
1.0	10.938694	2.0	13.332930
1.0	35.356149		
1.0	126.969556		
1.0	559.326258		
1.0	3719.607970		

ORBITAL ENERGIES, EIGENVECTORS

-32.71161	-1.89779	-0.78555
-0.016096	-0.679428	0.611545
0.060604	-0.439333	0.480481
0.549850	0.233495	0.129042
0.422651	0.121295	0.0
0.117891	0.028759	0.0
0.016758	0.003993	0.0

-32.75657	-1.90118	-0.78665
-0.008879	0.619267	0.611315
0.038154	0.509456	0.480681
0.448705	-0.197128	0.129109
0.456177	-0.142541	0.0
0.174895	-0.043138	0.0
0.038789	-0.009385	0.0
0.005193	-0.001211	0.0

NEON 8/3 DERIVED SET

TOTAL HF ENERGY
-0.12830852120 03

POTENTIAL ENERGY KINETIC ENERGY
-0.25661405660 03 0.12830553540 03

VIRIAL THEOREM
-0.20000232700 01

NEON 7/4 DERIVED SET

TOTAL HF ENERGY
-0.12845800510 03

POTENTIAL ENERGY KINETIC ENERGY
-0.25692511280 03 0.12846710770 0

VIRIAL THEOREM
-0.19999291450 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.502160	2.0	0.600310
1.0	1.711400	2.0	2.777120
1.0	9.446300	2.0	13.332900
1.0	27.484400		
1.0	85.675300		
1.0	304.018000		
1.0	1336.850000		
1.0	8905.070000		

S		P	
1.0	0.523730	2.0	0.432210
1.0	1.775050	2.0	1.697600
1.0	10.938700	2.0	6.230340
1.0	35.356100	2.0	28.436600
1.0	126.970000		
1.0	559.326000		
1.0	3719.610000		

ORBITAL ENERGIES,EIGENVECTORS

-32.76867	-1.90199	-0.78718
-0.005032	-0.589457	0.611206
0.025630	-0.543134	0.480777
0.362173	0.160170	0.129140
0.462958	0.158452	0.0
0.226525	0.056943	0.0
0.066169	0.016369	0.0
0.013456	0.003126	0.0
0.001756	0.000416	0.0

-32.75025	-1.91730	-0.83127
-0.008936	0.618657	0.456330
0.038353	0.510251	0.508562
0.448907	-0.197685	0.239750
0.455960	-0.142403	0.045966
0.174333	-0.043177	0.0
0.038779	-0.009396	0.0
0.005192	-0.001212	0.0

NEON 8/4 SOURCE SET

TOTAL HF ENERGY
-0.12848170320 03

POTENTIAL ENERGY -0.25696555810 03 KINETIC ENERGY 0.12848385490 03

VIRIAL THEOREM
-0.19999832530 01

NEON 9/4 DERIVED SET

TOTAL HF ENERGY
-0.12848873390 03

POTENTIAL ENERGY -0.25697622820 03 KINETIC ENERGY 0.12848749430 03

VIRIAL THEOREM
-0.20000096470 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.502159	2.0	0.432295
1.0	1.711440	2.0	1.697598
1.0	9.446346	2.0	6.280344
1.0	27.484367	2.0	28.436577
1.0	85.675282		
1.0	304.018339		
1.0	1336.848500		
1.0	8905.071356		

S		P	
1.0	0.481320	2.0	0.432210
1.0	1.632770	2.0	1.697600
1.0	7.601760	2.0	6.280340
1.0	19.488200	2.0	28.436600
1.0	53.293200		
1.0	161.629000		
1.0	566.110000		
1.0	2477.760000		
1.0	16501.200000		

ORBITAL ENERGIES, EIGENVECTORS,

-32.76237	-1.91815	-0.83179
-0.005072	-0.588776	0.456214
0.025785	-0.544043	0.508626
0.362434	0.160793	0.239800
0.462747	0.158308	0.045977
0.226439	0.056075	0.0
0.066149	0.016374	0.0
0.013453	0.003127	0.0
0.001755	0.000416	0.0

-32.76553	-1.91884	-0.83216
-0.001972	-0.557282	0.456159
0.014258	-0.573744	0.508657
0.242745	0.096923	0.239819
0.442024	0.177188	0.045978
0.301948	0.079744	0.0
0.116387	0.029774	0.0
0.031598	0.007382	0.0
0.006261	0.001496	0.0
0.000815	0.000190	0.0

NEON 9/5 SOURCE SET

TOTAL HF ENERGY
-0.12852822180 03

POTENTIAL ENERGY KINETIC ENERGY
-0.25705435090 03 0.12852612900 03

VIRIAL THEOREM
-0.20000162830 01

NEON 10/5 DERIVED SET

TOTAL HF ENERGY
-0.12853179900 03

POTENTIAL ENERGY KINETIC ENERGY
-0.25706680260 03 0.12853500370 03

VIRIAL THEOREM
-0.19999750670 01

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BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.481315	2.0	0.331057
1.0	1.632772	2.0	1.147741
1.0	7.601760	2.0	3.697860
1.0	19.488234	2.0	12.501192
1.0	53.293240	2.0	55.030482
1.0	161.623536		
1.0	566.109598		
1.0	2477.761790		
1.0	16501.214801		

S		P	
1.0	0.398940	2.0	0.331060
1.0	1.206600	2.0	1.147740
1.0	3.204770	2.0	3.697860
1.0	10.612500	2.0	12.501200
1.0	28.819600	2.0	55.030500
1.0	82.141200		
1.0	255.327000		
1.0	907.395000		
1.0	4000.200000		
1.0	26700.700000		

ORBITAL ENERGIES,EIGENVECTORS

-32.76823	-1.92535	-0.84476
-0.001975	-0.556735	0.333880
0.014270	-0.574413	0.485586
0.242826	0.097171	0.320808
0.441976	0.177145	0.106925
0.301929	0.079793	0.016995
0.116378	0.029773	0.0
0.031596	0.007386	0.0
0.006260	0.001496	0.0
0.000815	0.000190	0.0

-32.76884	-1.92685	-0.84526
0.002387	-0.406000	0.333862
-0.007421	-0.614162	0.485598
0.054451	-0.123218	0.320812
0.373971	0.187675	0.106920
0.424046	0.135069	0.016995
0.213976	0.056067	0.0
0.071212	0.017340	0.0
0.017952	0.004262	0.0
0.003467	0.000816	0.0
0.000447	0.000105	0.0

NEON 10/6 SOURCE SET

TOTAL HF ENERGY
-0.12854121790 03

POTENTIAL ENERGY	KINETIC ENERGY
-0.25708259890 03	0.12854138100 03

VIRIAL THEOREM
-0.19999987310 01

NEON 11/6 SOURCE SET

TOTAL HF ENERGY
-0.12854287920 03

POTENTIAL ENERGY	KINETIC ENERGY
-0.25708226740 03	0.12853938820 03

VIRIAL THEOREM
-0.20000271590 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.398940	2.0	0.258730
1.0	1.206600	2.0	0.803800
1.0	3.204770	2.0	2.346450
1.0	10.612500	2.0	6.831200
1.0	28.819600	2.0	22.235700
1.0	82.141200	2.0	95.811300
1.0	255.327000		
1.0	907.395000		
1.0	4000.200000		
1.0	26700.700000		

S		P	
1.0	0.336866	2.0	0.258728
1.0	0.929004	2.0	0.803801
1.0	2.415100	2.0	2.346453
1.0	8.144819	2.0	6.831199
1.0	20.265070	2.0	22.235709
1.0	52.422821	2.0	95.811320
1.0	146.138634		
1.0	450.723655		
1.0	1602.998594		
1.0	7066.927907		
1.0	47478.979673		

ORBITAL ENERGIES,EIGENVECTORS

-32.77081	-1.92931	-0.84903
0.002388	-0.405697	0.231036
-0.007426	-0.614472	0.433447
0.054463	-0.123204	0.370276
0.373977	0.187714	0.180537
0.424038	0.135080	0.048648
0.213972	0.056077	0.007005
0.071212	0.017361	0.0
0.017951	0.004263	0.0
0.003667	0.000816	0.0
0.000447	0.000105	0.0

-32.77177	-1.92960	-0.84920
0.001276	-0.285698	0.231036
-0.003398	-0.591967	0.433429
0.023593	-0.278379	0.370291
0.258600	0.135805	0.180539
0.423204	0.157148	0.049651
0.285129	0.078114	0.007006
0.118543	0.029915	0.0
0.036608	0.008719	0.0
0.008936	0.002122	0.0
0.001708	0.000400	0.0
0.000219	0.000052	0.0

NEON 12/6 DERIVED SET

TOTAL HF ENERGY
-0.1285436002D 03

POTENTIAL ENERGY	KINETIC ENERGY
-0.2570872200D 03	0.1285403198D 03

VIRIAL THEOREM
-0.2000023950 01

NEON 11/7 DERIVED SET

TOTAL HF ENERGY
-0.1285452207D 03

POTENTIAL ENERGY	KINETIC ENERGY
-0.2570974006D 03	0.1285421799D 03

VIRIAL THEOREM
-0.2000023656D 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.314860	2.0	0.258730
1.0	0.642450	2.0	0.803800
1.0	2.187020	2.0	2.346450
1.0	6.357450	2.0	6.831200
1.0	14.645000	2.0	22.235700
1.0	35.110400	2.0	95.811300
1.0	90.307400		
1.0	253.334000		
1.0	789.803000		
1.0	2830.330000		
1.0	12444.500000		
1.0	83539.600000		

S		P	
1.0	0.336870	2.0	0.206120
1.0	0.929000	2.0	0.579190
1.0	2.415100	2.0	1.554640
1.0	6.144820	2.0	4.118030
1.0	20.265100	2.0	11.422800
1.0	52.422800	2.0	36.454400
1.0	146.119000	2.0	155.151000
1.0	450.724000		
1.0	1603.000000		
1.0	7066.930000		
1.0	47479.000000		

ORBITAL ENERGIES, EIGENVECTORS

-32.77200	-1.92965	-0.84922
0.000391	-0.243871	0.231036
-0.000103	-0.574533	0.433425
0.010245	-0.336143	0.370294
0.155332	0.075234	0.130539
0.377580	0.164927	0.048651
0.343760	0.102184	0.007006
0.177714	0.046474	0.0
0.065182	0.015793	0.0
0.018753	0.004463	0.0
0.004434	0.001041	0.0
0.000940	0.000198	0.0
0.000108	0.000025	0.0

-32.77216	-1.93020	-0.85012
0.001276	-0.285630	0.150343
-0.003398	-0.592021	0.362671
0.023594	-0.278392	0.384734
0.258605	0.135816	0.251086
0.423200	0.157151	0.094494
0.285128	0.078116	0.023492
0.118542	0.029917	0.003157
0.036508	0.008719	0.0
0.008936	0.002172	0.0
0.001708	0.000400	0.0
0.000219	0.000052	0.0

NEON 12/7 SOURCE SET

TOTAL HF ENERGY
-0.12854574040 03

POTENTIAL ENERGY	KINETIC ENERGY
-0.25708881630 03	0.12854307580 03

VIRIAL THEOREM
-0.20000207290 01

NEON 13/7 DERIVED SET

TOTAL HF ENERGY
-0.12854596310 03

POTENTIAL ENERGY	KINETIC ENERGY
-0.25708971320 03	0.12854375010 03

VIRIAL THEOREM
-0.20000172160 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.314860	2.0	0.206120
1.0	0.842450	2.0	0.579190
1.0	2.187020	2.0	1.554640
1.0	6.357450	2.0	4.118030
1.0	14.645000	2.0	11.422800
1.0	35.110400	2.0	36.454400
1.0	90.307400	2.0	155.151000
1.0	253.338000		
1.0	787.700654		
1.0	2804.790709		
1.0	12390.008371		
1.0	83039.823436		

S		P	
1.0	0.295540	2.0	0.206120
1.0	0.765730	2.0	0.579190
1.0	1.936500	2.0	1.554640
1.0	4.965180	2.0	4.118030
1.0	11.015700	2.0	11.422800
1.0	24.862000	2.0	36.454400
1.0	59.389100	2.0	155.151000
1.0	153.471000		
1.0	436.513000		
1.0	1384.610000		
1.0	5060.150000		
1.0	23107.500000		
1.0	166165.000000		

ORBITAL ENERGIES,EIGENVECTORS

-32.77240	-1.93026	-0.85015
0.000392	-0.243807	0.150349
-0.000105	-0.574573	0.362663
0.010249	-0.336177	0.384738
0.155330	0.075252	0.251085
0.377689	0.164927	0.098495
0.343746	0.102185	0.023492
0.177729	0.044479	0.003157
0.065152	0.015786	0.0
0.018755	0.004477	0.0
0.004474	0.001051	0.0
0.000849	0.000200	0.0
0.000109	0.000025	0.0

-32.77249	-1.93029	-0.85016
0.000097	-0.207474	0.150353
0.000906	-0.546246	0.362659
0.003725	-0.381538	0.384740
0.084180	0.008830	0.251084
0.306175	0.157368	0.098495
0.369605	0.122137	0.023492
0.237714	0.065144	0.003157
0.104653	0.026006	0.0
0.035074	0.008437	0.0
0.009588	0.002262	0.0
0.002193	0.000517	0.0
0.000401	0.000094	0.0
0.000047	0.000011	0.0

NEON 13/8 SOURCE SET

TOTAL HF ENERGY
-0.12854657420 03

POTENTIAL ENERGY	KINETIC ENERGY
-0.25709172690 03	0.12854515270 03

VIRIAL THEOREM
-0.20000110590 01

NEON 14/8 DERIVED SET

TOTAL HF ENERGY
-0.12854667590 03

POTENTIAL ENERGY	KINETIC ENERGY
-0.25709217520 03	0.12854549930 03

VIRIAL THEOREM
-0.20000091530 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.295538	2.0	0.164627
1.0	0.765728	2.0	0.418788
1.0	1.936503	2.0	1.033764
1.0	4.965175	2.0	2.542082
1.0	11.015704	2.0	6.389537
1.0	24.861967	2.0	17.389549
1.0	59.389087	2.0	55.077385
1.0	153.471476	2.0	234.945000
1.0	436.512576		
1.0	1384.612313		
1.0	5060.153856		
1.0	23107.524226		
1.0	166165.080633		

S		P	
1.0	0.285620	2.0	0.164630
1.0	0.723060	2.0	0.418790
1.0	1.771300	2.0	1.033760
1.0	4.212820	2.0	2.542080
1.0	8.762750	2.0	6.389540
1.0	18.634400	2.0	17.389500
1.0	41.766300	2.0	55.077400
1.0	100.115000	2.0	234.945000
1.0	260.221000		
1.0	744.787000		
1.0	2399.530000		
1.0	9155.290000		
1.0	43638.300000		
1.0	279341.000000		

ORBITAL ENERGIES,EIGENVECTORS

-32.77248	-1.93038	-0.85035
0.000097	-0.207463	0.088172
0.000906	-0.546256	0.278054
0.003726	-0.381540	0.365458
0.084180	0.008834	0.306363
0.306176	0.157369	0.166455
0.369603	0.122136	0.056650
0.237716	0.065145	0.012496
0.104652	0.026005	0.001575
0.035074	0.008437	0.0
0.009588	0.002262	0.0
0.002193	0.000517	0.0
0.000401	0.000094	0.0
0.000047	0.000011	0.0

-32.77253	-1.93040	-0.85036
0.000138	-0.188524	0.088176
0.000647	-0.522247	0.278049
0.002901	-0.398055	0.365458
0.047252	-0.043650	0.306364
0.225886	0.132607	0.166455
0.359490	0.133940	0.056650
0.285730	0.083011	0.012496
0.148919	0.038215	0.001575
0.058547	0.014268	0.0
0.018590	0.004418	0.0
0.004970	0.001172	0.0
0.001090	0.000256	0.0
0.000180	0.000042	0.0
0.000023	0.000005	0.0

NEON 14/9 SOURCE SET

TOTAL HF ENERGY
-0.12854686480 03

POTENTIAL ENERGY	KINETIC ENERGY
-0.25709311070 03	0.12854624590 03

VIRIAL THEOREM
-0.20000048150 01

BASIS FUNCTIONS (PRINCIPAL QUANTUM NUMBER, ORBITAL EXPONENTS)

S		P	
1.0	0.285620	2.0	0.132290
1.0	0.723060	2.0	0.308830
1.0	1.771300	2.0	0.703960
1.0	4.212820	2.0	1.626530
1.0	8.762750	2.0	3.828170
1.0	18.634400	2.0	9.449440
1.0	41.766300	2.0	25.692900
1.0	100.115000	2.0	82.055200
1.0	260.221000	2.0	354.616931
1.0	744.787000		
1.0	2399.530000		
1.0	9155.291348		
1.0	43638.324426		
1.0	279341.011322		

ORBITAL ENERGIES,EIGENVECTORS

-32.77246	-1.93039	-0.85039
0.000138	-0.188528	0.046862
0.000647	-0.522245	0.195385
0.002901	-0.398056	0.319232
0.047253	-0.043646	0.330480
0.225866	0.132606	0.234654
0.359490	0.133940	0.108563
0.285729	0.083011	0.033016
0.148919	0.038215	0.006724
0.058547	0.014268	0.000783
0.018591	0.004418	0.0
0.004970	0.001172	0.0
0.001090	0.000256	0.0
0.000180	0.000042	0.0
0.000023	0.000005	0.0