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Tables of accurate STF HF wavefunctions from B to Ca

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Accurate Slater type function (STF) Hartree-Fock (HF) wavefunctions are calculated and tabled from B to Ca. The STF's have a form of $r^n e^{-\gamma r}$ and the powers (n) of r are carefully determined. The total atomic energies agree with those of numerical HF (NHF) within the error of 4×10^{-6} a.u. and 1×10^{-5} a.u. for B to F and for Ne to Ca, respectively. The STF HF basis sets given will be useful to benchmark calculations for the molecular, solid, and atomic electronic states. Applications of the STF HF basis to molecular calculations are given and briefly discussed. Sample calculations are performed on the N_2 and P_2 molecules.

Key words: Atomic Hartree-Fock — Slater-type function (STF)

1. Introduction

The ability of electronic computers improves year by year. Molecular electronic calculations and solid state calculations also attain higher quality. Many of these use Gaussian type functions (GTF's). Recently it has been found that a considerable number of polarization functions must be added to GTF basis sets to obtain reliable SCF molecular wavefunctions. However even though the accuracy of GTF calculations increases, we still worry about where the calculated results converge. Questions arise from the inaccurate behaviour of GTF's near the nucleus and at points far from the nucleus.

Here we use Slater type functions (STF's) and generate near HF wavefunctions by the method of Roothaan and Bagus [1]. We hope that such near HF wavefunctions can be used to provide a benchmark for atomic and molecular electronic calculations, as well as solid state calculations.

2. Previous work

There have appeared many STF SCF wavefunctions [2-9]. Using even-tempered basis sets (1s and 2p STF's) where the two non-linear parameters α and β were variationally determined, Raffenetti [7] has given reasonably correct total energies (TE's) for Li to Ca. Among others, Clementi and Roetti [8] have compiled the atomic SCF wavefunctions from He to Xe. They have calculated the ground, excited, and even ionized states. Their results are often referred as accurate HF. There are, however, small differences between the TE's of numerical HF (NHF) [10, 11] and the analytic expansion results of Clementi and Roetti [8] as will be soon discussed.

Schmidt and Ruedenberg [12] have shown that the true HF limit can be obtained by the analytic expansion method using systematically large even-tempered basis sets. One of the present authors (HT) [9] has analyzed the results of Clenentti and Roetti [8], Bagus et al. [3], and Huzinaga [13, 14] and has found that the three 1s STF's are necessary to get near HF wavefunctions for the second row atoms from Li to Ne.

3. Present work

Raffenetti and Ruedenberg [7], in their work with even tempered STF's, have shown that excellent wavefunctions can be obtained using exponential primitives of the 1s, 2p, 3d type only. In a previous work [9] we have further pursued this approach but without the eventempered exponent constraint.

The present study is an extension of this work.

We have, here, carefully chosen the power(n) of r in STF's, $r^n e^{-\gamma r}$. It is found that the use of 1s and 2p STF's for the second row atoms leads to a considerable TE lowering compared with other calculations. As will be shown, five 1s and five 2p STF's supply almost accurate HF TE's. On the other hand, tests of the set of this type on Cl ^{2}P provided negative results. A linear dependence occurred and the efficiency of this type of set is decreased: the use of seven 1s and seven 2p for Cl gives a TE of −459.481970 a.u. which is lower than that of CR by 0.0001 a.u. The use of seven 1s and eight 2p functions gives −459.482010 a.u., while eight 1s and eight 2p lead to slight linear dependence and give almost the same energy of −459.482017 a.u. (The nearest two exponents in 1s STF's are 4.3918 (ζ_5) and 3.5085 (ζ_6) and the overlap integral between the two is 0.9813. The two STF's have rather large amplitude with opposite sign in the HF 2S and 3S orbitals; $C_{\zeta 5}$ and $C_{\zeta 6}$ in 2S and 3S are (−2.49, 0.95) and (0.30, −1.93), respectively.) The best set that we found was composed of two 1s, seven 2s and eight 2p STF's. This set gives a TE of −459.482063 a.u., quite close to that of NHF (−459.48207 a.u.). This expansion pattern has been used throughout the third row atoms. Details will be given elsewhere [15].

The TE's calculated by various authors for Li to Ne and Na to Ca are collected in Tables 1-2 for a quick review. The NHF results of Fischer [10] are also shown in these tables for comparison. Tatewaki [9] has found TE of −99.409340 a.u.

for F ^2P, using five 1s and four 2p, while the NHF value is −99.409349 a.u. The extra 2p STF added in this work considerably reduces the error, resulting in a TE of −99.409346 a.u. As a whole, the present analytic sets give an error in TE's of less than 4×10^{-6} a.u. for *B* to Ne (Instead of the result of NHF, we have adopted that of large even-tempered set as 'exact' value for Ne [7]: see Table 1). The error is somewhat larger for Na to Ca, i.e., about 1×10^{-5} a.u. TE's given by Clementi and Roetti and others are reasonably close to those of NHF for the atoms with a smaller nuclear charge except for those of Raffenetti who imposed the even-tempered constraint. For heavy atoms (P−Ca) the difference between the analytic HF of Clementi and Roetti and NHF becomes a little larger. Examples of the orbital energies (ε's) for fluorine $(2s^22p^5)$ ^2P and chlorine $(3s^23p^5)$ ^2P are shown in Table 3. Good agreement is observed in the orbital energies of the present HF and NHF of Fischer [10]. The exponents and expansion coefficients for B to CA are summarized in Table 4. The expectation values $\langle r^n \rangle$ for $n=-3$, −2, −1, 0, 1, and 2 are also shown in this table. There exist close agreement among the NHF values of Fischer [10], the best Raffenetti-Ruedenberg's values [7b], and the present results.

The atomic SCF wavefunctions have been used in molecular SCF calculations on the N_2 and P_2 molecules. Many sets of the polarization functions are added

Table 1. Comparison of the total energies (with sign reversed) of B to Ne by various basis sets

	Li	Be	B	C
R[a]	7.432720	14.573015	24.529049	37.688598
CR[b]	7.432726	14.573021	24.529057	37.688612
BGR[c]	7.432726	14.573021	24.529058	37.688615
T[d]	7.432726	14.573019	24.529056	37.688612
T[e]	7.432725	14.573020	24.529057	37.688616
P[f]			24.529057	37.688616
Exact[g]	7.432727	14.573023	24.529061	37.688619
	N	**O**	**F**	**Ne**
R	54.400895	74.809286	99.409204	128.54695
CR	54.400924	74.809370	99.409300	128.54705
BGR	54.400926	74.809384	99.409327	128.54707
T	54.400926	74.809384	99.409331	128.54707
T'	54.400930	74.809393	99.409340	128.54709
P	54.400931	74.809395	99.409346	128.547094
Exact	54.400934	74.809398	99.409349	128.547097

[a] See [7]; the basis sets are composed of six 1s and four 2p STF's

[b] See [8]; the basis sets are composed of two 1s, four 2s, and four 2p STF's

[c] See [3]; the basis sets are composed of two 1s, two 2s, one 3s, and four 2p STF's

[d] See [9]; the basis sets are composed of three 1s, two 2s, and four 2p STF's

[e] See [9]; the basis sets are composed of five 1s and four 2p STF's

[f] Present work; the basis sets are composed of five 1s and five 2p STF's

[g] From Li to F, the exact values are the results of NHF [10], while that for Ne is the result of large even-tempered STF's [7]

Table 2. Comparison of the total energies (with sign reversed) of Na to Ca by various basis sets

	Na	Mg	Al	Si	P
R[a]	161.85880	199.61455	241.87663	288.85428	340.71870
CR[b]	161.85890	199.61461	241.87668	288.85431	340.71869
H[c]	161.85889	199.61461	241.87669	288.85434	340.71876
P[d]	161.85891	199.61462	241.87670	288.85436	340.71878
NHF[e]	161.85891	199.61463	241.87671	288.85436	340.71878
	S	Cl	Ar	K	Ca
R	397.50477	459.48180	526.81702	599.16457	676.75715
CR	397.50485	459.48187	526.81739	599.16453	676.75803
H	397.50487	459.48204	526.81748		
P	397.50489	459.48206	526.81750	599.16478	676.75817
NHF	397.50490	459.48207	526.81751	599.16479	676.75818

[a] See [7]; for third row atoms, the basis sets are domposed of nine 1s and six 2p STF's

[b] See [8]; the basis sets are composed of one 1s, seven 3s, one 2p, and seven 4p STF's except for Na and Mg, where seven 2p are replaced by four 2p STF's. For K and Ca, they are composed of two 1s, two 2s, three 3s, four 4s, two 2p, and four 3p STF's

[c] See [5]; expansion patterns of STF's are the same as [b]

[d] Present work; for third row atoms, the basis sets are composed of two 1s, seven 2s. and eight 2p STF's except for Na and Mg where eight 2p are replaced by five 2p STF's. For K and Ca, they are composed of two 1s, two 2s, eight 3s, and eight 2p STF's

[e] See [10]

Table 3. Comparison of the orbital energies (with sign reversed) of F and Cl

	Fluorine CR[a]	$K^2\ 2s^22p^5$ 2P BGR[b]	P[c]	NHF[d]
TE	99.409300	99.409327	99.409346	99.409349
ε_{1s}	26.38273	26.38265	26.38277	26.38276
ε_{2s}	1.57254	1.57245	1.57254	1.57253
ε_{2p}	0.83001	0.72994	0.73002	0.73002
	Chlorine CR[a]	$K^2L^83s^23p^{52}P$ H[e]	P[c]	NHF[d]
TE	459.48187	459.48204	459.48206	459.58207
ε_{1s}	104.88469	104.88440	104.88441	104.88442
ε_{2s}	10.60777	10.60747	10.60748	10.60748
ε_{3s}	1.07311	1.07290	1.07291	1.07291
ε_{2p}	8.07252	8.07222	8.07223	8.07222
ε_{3p}	0.50652	0.50639	0.50640	0.50640

[a] See [8]

[b] See [3]

[c] Present work

[d] See [10]

[e] See [5]

Table 4. The STF HF wavefunctions from B to Ca

B K(2) 2S*2 2P*1 (2P)

Total Energy -24. 529057

Orbital Symmetry		1S	2S			2P
Orbital Energy		-7. 69533	-0. 49470			-0. 30986
Exponent		Coefficients		Exponent		Coefficients
1s	8. 03262	0. 07181	0. 01429	2p	5. 82091	0. 00723
1s	4. 47655	0. 91904	0. 07208	2p	2. 50711	0. 07695
1s	2. 70048	0. 01893	0. 50042	2p	1. 54122	0. 32283
1s	1. 19529	-0. 00025	0. 39619	2p	0. 94263	0. 60077
1s	0. 99407	0. 00041	-1. 65353	2p	0. 69869	0. 05678
<R** 0>		1. 00000	1. 00000			1. 00000
<R**-3>						0. 77569
<R**-2>		44. 54236	2. 02555			0. 52989
<R**-1>		4. 67434	0. 71288			0. 60501
<R** 1>		0. 32587	1. 97707			2. 20476
<R** 2>		0. 14336	4. 70916			6. 14607
Rmax		0. 21100	1. 52544			1. 58600

C K(2) 2S*2 2P*2 (3P)

Total Energy -37. 688616

Orbital Symmetry		1S	2S			2P
Orbital Energy		-11. 32551	-0. 70563			-0. 43334
Exponent		Coefficients		Exponent		Coefficients
1s	9. 66836	0. 06165	0. 01250	2p	7. 07990	0. 00696
1s	5. 48751	0. 91888	0. 06698	2p	3. 04833	0. 11182
1s	3. 43184	0. 02797	0. 52109	2p	1. 85359	0. 38038
1s	1. 55063	0. 00033	0. 07211	2p	1. 14016	0. 53936
1s	1. 19048	0. 00041	-1. 33646	2p	0. 80298	0. 03282
<R** 0>		1. 00000	1. 00000			1. 00000
<R**-3>						1. 69201
<R**-2>		65. 23976	3. 25672			0. 89207
<R**-1>		5. 66444	0. 89680			0. 78350
<R** 1>		0. 26844	1. 58934			1. 71449
<R** 2>		0. 09720	3. 05201			3. 74678
Rmax		0. 17440	1. 22221			1. 21124

Table 4 (continued)

```
                         N      K(2) 2S*2 2P*3 (4S)

                                Total Energy -54. 400931

Orbital Symmetry     1S            2S                                2P

Orbital Energy    -15. 62906    -0. 94532                        -0. 56759

  Exponent        Coefficients                   Exponent       Coefficients

 1s   11. 28894     0. 05421      0. 01091      2p     8. 25307     0. 00681
 1s    6. 50357     0. 91628      0. 06321      2p     3. 60392     0. 13653
 1s    4. 15941     0. 03731      0. 53270      2p     2. 17162     0. 41100
 1s    1. 50925     0. 00138     -0. 32768      2p     1. 33358     0. 49463
 1s    1. 36560    -0. 00033     -0. 93891      2p     0. 92006     0. 02713

      <R** 0>       1. 00000      1. 00000                          1. 00000
      <R**-3>                                                       3. 09990
      <R**-2>      89. 84849      4. 75496                          1. 33629
      <R**-1>       6. 65324      1. 07818                          0. 95769
      <R** 1>       0. 22830      1. 33228                          1. 40963
      <R** 2>       0. 07027      2. 14940                          2. 54765
       Rmax         0. 14862      1. 02180                          0. 98327


                         O      K(2) 2S*2 2P*4 (3P)

                                Total Energy -74. 809395

Orbital Symmetry     1S            2S                                2P

Orbital Energy    -20. 66866    -1. 24432                        -0. 63191

  Exponent        Coefficients                   Exponent       Coefficients

 1s   12. 89105     0. 04872      0. 00964      2p     9. 53550     0. 00602
 1s    7. 51818     0. 91472      0. 06129      2p     4. 18065     0. 15685
 1s    4. 86264     0. 04380      0. 55082      2p     2. 51031     0. 40778
 1s    1. 91655     0. 00086     -0. 31349      2p     1. 50781     0. 45175
 1s    1. 56389     0. 00043     -0. 96360      2p     1. 08528     0. 06606

      <R** 0>       1. 00000      1. 00000                          1. 00000
      <R**-3>                                                       4. 97438
      <R**-2>     118. 39021      6. 59284                          1. 81872
      <R**-1>       7. 64217      1. 26527                          1. 11111
      <R** 1>       0. 19859      1. 14196                          1. 23220
      <R** 2>       0. 05315      1. 58116                          1. 97497
       Rmax         0. 12949      0. 87554                          0. 83261
```

Table 4 (continued)

F K(2) 2S*2 2P*5 (2P)

Total Energy -99.409346

Orbital Symmetry		1S	2S			2P
Orbital Energy		-26.38277	-1.57254			-0.73002
Exponent		Coefficients		Exponent		Coefficients
1s	14.50029	0.04402	0.00847	2p	10.72879	0.00561
1s	8.53821	0.91232	0.05962	2p	4.76849	0.16970
1s	5.57342	0.05054	0.56052	2p	2.83521	0.41836
1s	2.17914	0.00090	-0.42942	2p	1.67212	0.43530
1s	1.74367	0.00055	-0.85172	2p	1.17787	0.06614
<R** 0>		1.00000	1.00000			1.00000
<R**-3>						7.54546
<R**-2>		150.84325	8.69848			2.39477
<R**-1>		8.63036	1.44975			1.27167
<R** 1>		0.17575	1.00109			1.08478
<R** 2>		0.04161	1.21651			1.54352
Rmax		0.11472	0.76699			0.71982

Ne K(2) 2S*2 2P*6 (1S)

Total Energy -128.54709

Orbital Symmetry		1S	2S			2P
Orbital Energy		-32.77242	-1.93038			-0.85040
Exponent		Coefficients		Exponent		Coefficients
1s	16.02696	0.04119	0.00763	2p	11.71898	0.00569
1s	9.55386	0.90946	0.05772	2p	5.32678	0.18193
1s	6.28932	0.05586	0.56648	2p	3.15883	0.41875
1s	2.44327	0.00120	-0.49266	2p	1.87553	0.40602
1s	1.92513	0.00048	-0.78978	2p	1.33620	0.08656
<R** 0>		1.00000	1.00000			1.00000
<R**-3>						10.90630
<R**-2>		187.20677	11.07259			3.05884
<R**-1>		9.61805	1.63255			1.43535
<R** 1>		0.15763	0.89211			0.96527
<R** 2>		0.03347	0.96704			1.22845
Rmax		0.10297	0.68291			0.63396

Table 4 (continued)

Na K(2) L(8) 3S*1 (2S)

Total Energy -161.85891

Orbital Symmetry		1S	2S	3S
Orbital Energy		-40.47850	-2.79702	-0.18210
Exponent		Coefficients		
1s	16.21190	0.06724	0.01151	0.00227
1s	10.24827	0.93757	0.23881	0.03484
2s	8.71557	-0.01490	0.15601	0.02863
2s	6.46001	0.02068	-0.16162	-0.03148
2s	3.87388	-0.00497	-0.55239	-0.07603
2s	2.69135	0.00328	-0.46349	-0.09947
2s	1.48361	-0.00081	0.00024	-0.12017
2s	0.69128	0.00068	-0.00102	0.55487
2s	0.58975	-0.00047	0.00044	0.54094
	<R** 0>	1.00000	1.00000	1.00000
	<R**-2>	227.53589	14.45473	0.39849
	<R**-1>	10.60738	1.86734	0.30140
	<R** 1>	0.14286	0.77907	4.20874
	<R** 2>	0.02748	0.73150	20.70611
	Rmax	0.09340	0.60774	3.39338

Orbital Symmetry		2P
Orbital Energy		-1.51814
Exponent		Coefficients
2p	12.54752	0.00661
2p	5.77218	0.22345
2p	3.34436	0.46916
2p	2.13398	0.37549
2p	1.13450	0.00506
	<R** 0>	1.00000
	<R**-3>	17.00503
	<R**-2>	4.18770
	<R**-1>	1.69660
	<R** 1>	0.79849
	<R** 2>	0.82214
	Rmax	0.54899

Table 4 (continued)

Mg K(2) L(8) 3S*2 (1S)

Total Energy -199.61462

Orbital Symmetry		1S	2S	3S
Orbital Energy		-49.03173	-3.76772	-0.25305
Exponent		Coefficients		
1s	18.10400	0.05259	-0.00941	-0.00300
1s	11.37501	0.94085	-0.24560	-0.04498
2s	9.80673	0.00262	-0.14598	-0.03774
2s	6.96475	0.01562	0.14110	0.04515
2s	4.21956	-0.00502	0.62098	0.07241
2s	3.03050	0.00391	0.40314	0.18780
2s	1.87539	-0.00117	-0.00916	0.09784
2s	0.98058	0.00045	0.00274	-0.57664
2s	0.71506	-0.00020	-0.00114	-0.55072
	<R** 0>	1.00000	1.00000	1.00000
	<R**-2>	271.85231	18.38414	0.78878
	<R**-1>	11.59795	2.10782	0.39939
	<R** 1>	0.13059	0.69034	3.25302
	<R** 2>	0.02296	0.57109	12.42160
	Rmax	0.08546	0.54641	2.58872

Orbital Symmetry		2P
Orbital Energy		-2.28222
Exponent		Coefficients
2p	14.26715	0.00546
2p	6.46220	0.22660
2p	3.69076	0.53108
2p	2.48162	0.30134
2p	1.30593	0.00377
	<R** 0>	1.00000
	<R**-3>	24.92220
	<R**-2>	5.46984
	<R**-1>	1.95169
	<R** 1>	0.68500
	<R** 2>	0.59770
	Rmax	0.48374

Table 4 (continued)

```
                    Al    K(2) L(8) 3S*2 3P*1 (2P)

                         Total Energy -241. 87670

Orbital Symmetry    1S              2S              3S

Orbital Energy   -58. 50101      -4. 91066       -0. 39341

 Exponent        Coefficients

1s  20. 37927      0. 03711      -0. 00691        0. 00168
1s  12. 56054      0. 94236      -0. 25066        0. 05770
2s  10. 86027      0. 02221      -0. 14486        0. 03653
2s   7. 43594      0. 01156       0. 13250       -0. 03047
2s   4. 54139     -0. 00580       0. 71286       -0. 18700
2s   3. 26954      0. 00903       0. 36011        0. 11444
2s   2. 75898     -0. 00543      -0. 06041       -0. 45667
2s   1. 59978      0. 00050       0. 00255        0. 36408
2s   0. 97370     -0. 00009      -0. 00016        0. 87617

    <R** 0>        1. 00000       1. 00000        1. 00000
    <R**-2>      320. 13921      22. 79981        1. 35956
    <R**-1>       12. 58925       2. 34901        0. 50679
    <R** 1>        0. 12026       0. 62003        2. 59909
    <R** 2>        0. 01946       0. 45890        7. 88772
     Rmax          0. 07876       0. 49607        2. 09779

Orbital Symmetry    2P              3P

Orbital Energy    -3. 21829      -0. 20995

 Exponent        Coefficients

2p  16. 46789      0. 00371      -0. 00051
2p   7. 46240      0. 18470      -0. 03369
2p   4. 42178      0. 49825      -0. 09739
2p   2. 93569      0. 45558       0. 07579
2p   2. 56805     -0. 09118      -0. 24234
2p   1. 47973      0. 00984       0. 01593
2p   1. 02442     -0. 00183       0. 30484
2p   0. 69302      0. 00054       0. 77163

    <R** 0>        1. 00000       1. 00000
    <R**-3>       34. 94033       1. 08801
    <R**-2>        6. 91587       0. 31055
    <R**-1>        2. 20511       0. 37929
    <R** 1>        0. 60054       3. 43370
    <R** 2>        0. 45536      14. 00317
     Rmax          0. 43229       2. 68609
```

Table 4 (continued)

Si K(2) L(8) 3S*2 3P*2 (3P)

Total Energy -288.85436

Orbital Symmetry		1S	2S	3S
Orbital Energy		-68.81245	-6.15654	-0.53984
Exponent		Coefficients		
1s	21.83699	0.03578	-0.00667	0.00226
1s	13.56225	0.94378	-0.25708	0.06474
2s	11.77293	0.02095	-0.14819	0.04498
2s	8.25260	0.01260	0.11482	-0.03982
2s	5.00111	-0.00735	0.72784	-0.14155
2s	3.82025	0.01016	0.30865	-0.09189
2s	3.19108	-0.00510	-0.00405	-0.29481
2s	1.61825	0.00039	0.00075	0.51613
2s	1.10992	-0.00012	0.00022	0.69766
	<R** 0>	1.00000	1.00000	1.00000
	<R**-2>	372.39206	27.69355	1.99823
	<R**-1>	13.58115	2.59040	0.60323
	<R** 1>	0.11143	0.56294	2.20708
	<R** 2>	0.01670	0.37726	5.67612
	Rmax	0.07304	0.45410	1.79826

Orbital Symmetry		2P	3P
Orbital Energy		-4.25605	-0.29711
Exponent		Coefficients	
2p	17.94393	0.00342	-0.00055
2p	8.12062	0.18893	-0.04061
2p	4.77793	0.54403	-0.13269
2p	3.34833	0.35036	0.27667
2p	3.04173	-0.03770	-0.48620
2p	1.75161	0.00330	0.12359
2p	1.07563	0.00087	0.55367
2p	0.80782	-0.00006	0.46776
	<R** 0>	1.00000	1.00000
	<R**-3>	47.27047	2.05362
	<R**-2>	8.52035	0.50119
	<R**-1>	2.45638	0.47803
	<R** 1>	0.53541	2.75222
	<R** 2>	0.35968	8.98088
	Rmax	0.39064	2.16974

Table 4 (continued)

```
                    P     K(2) L(8) 3S*2 3P*3 (4S)

                          Total Energy -340. 71878

Orbital Symmetry     1S             2S             3S

Orbital Energy     -79. 96972     -7. 51110      -0. 69642

  Exponent         Coefficients

 1s   23. 28241      0. 03427     -0. 00662       0. 00254
 1s   14. 60718      0. 94157     -0. 26111       0. 07031
 2s   12. 83904      0. 02636     -0. 14133       0. 04651
 2s    8. 55738      0. 01122      0. 10509      -0. 04333
 2s    5. 29637     -0. 00572      0. 88097      -0. 14079
 2s    3. 74632      0. 00817      0. 17916      -0. 50362
 2s    3. 12374     -0. 00497     -0. 02930       0. 12588
 2s    1. 71750      0. 00059      0. 00212       0. 63068
 2s    1. 23484     -0. 00019     -0. 00003       0. 55661

     <R** 0>         1. 00000      1. 00000       1. 00000
     <R**-2>       428. 61611     33. 05937       2. 71320
     <R**-1>        14. 57355      2. 83171       0. 69473
     <R** 1>         0. 10380      0. 51566       1. 93269
     <R** 2>         0. 01449      0. 31592       4. 34719
      Rmax           0. 06811      0. 41865       1. 58502

Orbital Symmetry     2P             3P

Orbital Energy      -5. 40096     -0. 39171

  Exponent         Coefficients

 2p   19. 20061      0. 00327     -0. 00050
 2p    8. 77890      0. 19168     -0. 04716
 2p    5. 08157      0. 64829     -0. 14527
 2p    3. 30529      0. 49130      0. 21645
 2p    3. 13622     -0. 29106     -0. 47906
 2p    1. 82115      0. 00449      0. 30311
 2p    1. 11523     -0. 00004      0. 75586
 2p    0. 84686     -0. 00000      0. 13610

     <R** 0>         1. 00000      1. 00000
     <R**-3>        62. 14771      3. 30974
     <R**-2>        10. 28402      0. 71574
     <R**-1>         2. 70627      0. 57015
     <R** 1>         0. 48340      2. 32272
     <R** 2>         0. 29180      6. 38968
      Rmax           0. 35633      1. 84332
```

Table 4 (continued)

S K(2) L(8) 3S*2 3P*4 (3P)

Total Energy -397.50489

Orbital Symmetry		1S	2S	3S
Orbital Energy		-92.00445	-9.00429	-0.87953
Exponent		Coefficients		
1s	24.93347	0.03092	-0.00655	0.00238
1s	15.66948	0.94135	-0.26407	0.07570
2s	13.84637	0.03006	-0.14451	0.04862
2s	9.67844	0.01014	0.07500	-0.02982
2s	5.77321	-0.00257	0.93985	-0.18961
2s	3.91743	0.00334	0.14164	-0.59582
2s	2.98704	-0.00206	-0.02214	0.31662
2s	1.78527	0.00054	0.00406	0.71276
2s	1.33766	-0.00020	-0.00057	0.39351
	<R** 0>	1.00000	1.00000	1.00000
	<R**-2>	488.81607	38.90285	3.53495
	<R**-1>	15.56645	3.07320	0.78610
	<R** 1>	0.09715	0.47577	1.72072
	<R** 2>	0.01269	0.26853	3.44321
	Rmax	0.06378	0.38828	1.42033

Orbital Symmetry		2P	3P
Orbital Energy		-6.68251	-0.43737
Exponent		Coefficients	
2p	20.13311	0.00336	0.00052
2p	9.40449	0.19531	0.05181
2p	5.40460	0.73186	0.16179
2p	3.08231	0.34713	1.00069
2p	2.83402	-0.24522	-0.91805
2p	1.57209	0.02373	-0.36813
2p	1.25865	-0.01565	-0.32666
2p	1.00074	0.00404	-0.33579
	<R** 0>	1.00000	1.00000
	<R**-3>	79.77736	4.83797
	<R**-2>	12.20277	0.94190
	<R**-1>	2.95445	0.65067
	<R** 1>	0.44104	2.06072
	<R** 2>	0.24209	5.06526
	Rmax	0.32760	1.61500

Table 4 (continued)

Cl K(2) L(8) 3S*2 3P*5 (2P)

Total Energy -459.48206

Orbital Symmetry		1S	2S	3S
Orbital Energy		-104.88441	-10.60748	-1.07291
Exponent		Coefficients		
1s	25.55717	0.03813	-0.00892	-0.00360
1s	16.57604	0.93831	-0.26646	-0.07890
2s	15.06005	0.02416	-0.12970	-0.04676
2s	9.67065	0.01356	0.04291	0.02823
2s	6.30827	-0.00744	0.91874	0.13216
2s	4.58325	0.00580	0.16437	0.59248
2s	3.15195	-0.00244	-0.00604	-0.25406
2s	1.91579	0.00078	0.00324	-0.82723
2s	1.41161	-0.00027	-0.00035	-0.26897
	<R** 0>	1.00000	1.00000	1.00000
	<R**-2>	552.98665	45.21102	4.43497
	<R**-1>	16.55969	3.31440	0.87488
	<R** 1>	0.09130	0.44171	1.55563
	<R** 2>	0.01120	0.23119	2.81299
	Rmax	0.05997	0.36203	1.28889

Orbital Symmetry		2P	3P
Orbital Energy		-8.07223	-0.50640
Exponent		Coefficients	
2p	19.52090	0.00489	0.00084
2p	9.90053	0.20176	0.05721
2p	5.81077	0.73913	0.15724
2p	3.70603	0.11590	0.52911
2p	3.08709	-0.02235	-0.43923
2p	1.67537	0.00129	-0.57845
2p	1.14799	0.00322	-0.34850
2p	1.07997	-0.00203	-0.10325
	<R** 0>	1.00000	1.00000
	<R**-3>	100.38885	6.76572
	<R**-2>	14.27777	1.20110
	<R**-1>	3.20154	0.73329
	<R** 1>	0.40572	1.84203
	<R** 2>	0.20433	4.05923
	Rmax	0.30322	1.43918

Table 4 (continued)

Ar K(2) L(8) 3S*2 3P*6 (1S)

Total Energy -526.81750

Orbital Symmetry		1S	2S	3S
Orbital Energy		-118.61035	-12.32215	-1.27735
Exponent		Coefficients		
1s	27.80172	0.02889	-0.00749	-0.00281
1s	17.76447	0.93772	-0.26770	-0.08275
2s	16.12769	0.03485	-0.13276	-0.04756
2s	11.31732	0.01149	0.01489	0.01068
2s	6.80847	-0.00267	0.95419	0.17715
2s	4.88518	0.00242	0.15289	0.59920
2s	3.22083	-0.00114	-0.00390	-0.34863
2s	2.02452	0.00045	0.00307	-0.81654
2s	1.51635	-0.00017	-0.00025	-0.20941
	<R** 0>	1.00000	1.00000	1.00000
	<R**-2>	621.13444	51.98402	5.41487
	<R**-1>	17.55323	3.55532	0.96198
	<R** 1>	0.08610	0.41228	1.42217
	<R** 2>	0.00996	0.20123	2.35043
	Rmax	0.05659	0.33924	1.18259

Orbital Symmetry		2P	3P
Orbital Energy		-9.57147	-0.59102
Exponent		Coefficients	
2p	20.12646	0.00529	0.00091
2p	10.55722	0.19682	0.05830
2p	6.27763	0.74812	0.15103
2p	4.21625	0.08215	0.52214
2p	3.47821	0.00726	-0.40381
2p	1.88774	-0.00461	-0.58652
2p	1.33207	0.00863	-0.13235
2p	1.21882	-0.00569	-0.32803
	<R** 0>	1.00000	1.00000
	<R**-3>	124.36739	8.97090
	<R**-2>	16.52544	1.47359
	<R**-1>	3.44999	0.81407
	<R** 1>	0.37533	1.66296
	<R** 2>	0.17434	3.31084
	Rmax	0.28215	1.29971

Table 4 (continued)

K K(2) L(8) 3S*2 3P*6 4S*1 (2S)

Total Energy -599.16478

Orbital Symmetry		1S	2S	3S	4S
Orbital Energy		-133.53303	-14.48995	-1.74878	-0.14747
Exponent		Coefficients			
1s	28.79450	0.03270	-0.00831	-0.00418	-0.00126
1s	18.64349	0.94123	-0.27250	-0.08704	-0.01595
2s	17.24525	0.02481	-0.12046	-0.05023	-0.01175
2s	10.24779	0.01757	0.42289	0.16730	0.03663
3s	9.64305	-0.00983	0.28686	0.05771	0.00165
3s	7.51731	0.00413	0.44395	0.29679	0.07209
3s	4.12168	-0.00185	0.03820	-0.14078	-0.06540
3s	3.34146	0.00145	-0.02015	-0.52799	-0.06643
3s	2.33470	-0.00036	0.00473	-0.47920	-0.15356
3s	1.07762	0.00008	-0.00079	-0.00381	0.08212
3s	0.70250	-0.00007	0.00062	0.00089	0.80550
3s	0.50895	0.00003	-0.00024	-0.00043	0.17178
	<R** 0>	1.00000	1.00000	1.00000	1.00000
	<R**-2>	693.27683	59.26679	6.81864	0.29540
	<R**-1>	18.54736	3.79770	1.07486	0.23659
	<R** 1>	0.08147	0.38639	1.27706	5.24384
	<R** 2>	0.00891	0.17659	1.88348	31.55105
	Rmax	0.05357	0.31895	1.08177	4.34722

Orbital Symmetry		2P	3P
Orbital Energy		-11.51928	-0.95442
Exponent		Coefficients	
2p	24.65683	0.00240	0.00039
2p	11.72499	0.16616	0.05204
2p	6.89687	0.76145	0.18437
2p	4.39728	0.13810	0.75178
2p	3.75438	-0.03063	-0.69067
2p	2.91836	-0.00396	0.05452
2p	1.93217	0.00264	-0.88048
2p	1.31324	-0.00054	-0.15348
	<R** 0>	1.00000	1.00000
	<R**-3>	151.80954	12.95203
	<R**-2>	18.92678	1.94645
	<R**-1>	3.69703	0.93901
	<R** 1>	0.34943	1.43685
	<R** 2>	0.15080	2.44065
	Rmax	0.26380	1.16218

Table 4 (continued)

Ca K(2) L(8) 3S*2 3P*6 4S*2 (1S)

Total Energy -676.75817

Orbital Symmetry		1S	2S	3S	4S
Orbital Energy		-149.36372	-16.82273	-2.24537	-0.19553
Exponent		Coefficients			
1s	29.61078	0.03818	-0.00956	0.00540	-0.00162
1s	19.42510	0.94864	-0.27828	0.09203	-0.02136
2s	18.21865	0.00764	-0.11396	0.05220	-0.01397
2s	10.82411	0.02151	0.41816	-0.17726	0.04565
3s	10.29046	-0.01276	0.28680	-0.05120	0.00473
3s	8.01725	0.00518	0.44664	-0.33082	0.09355
3s	4.53259	-0.00181	0.02992	0.21732	-0.08144
3s	3.32037	0.00141	-0.01192	0.66074	-0.13372
3s	2.46463	-0.00056	0.00445	0.28550	-0.17356
3s	1.12279	0.00011	-0.00069	-0.00089	0.44599
3s	0.75142	-0.00008	0.00049	0.00075	0.64251
3s	0.51054	0.00002	-0.00015	-0.00025	0.01768
	<R** 0>	1.00000	1.00000	1.00000	1.00000
	<R**-2>	769.40318	67.04739	8.40002	0.53514
	<R**-1>	19.54194	4.04086	1.18877	0.29974
	<R** 1>	0.07730	0.36350	1.15942	4.21843
	<R** 2>	0.00802	0.15617	1.54601	20.45286
	Rmax	0.05086	0.30092	0.99631	3.47540

Orbital Symmetry		2P	3P
Orbital Energy		-13.62926	-1.34070
Exponent		Coefficients	
2p	25.17785	0.00262	-0.00042
2p	12.37123	0.16485	-0.05607
2p	7.33368	0.78177	-0.16884
2p	5.21639	-0.02475	-0.66092
2p	4.74252	0.11802	0.37372
2p	2.99163	-0.01302	0.18820
2p	2.13061	0.00464	0.91891
2p	1.30881	-0.00061	0.06087
	<R** 0>	1.00000	1.00000
	<R**-3>	183.00450	17.73475
	<R**-2>	21.49123	2.46233
	<R**-1>	3.94409	1.05881
	<R** 1>	0.32687	1.27455
	<R** 2>	0.13173	1.90806
	Rmax	0.24770	1.05295

in order to see the convergence of TE. Here we only summarize the results of the largest basis set;

1) TE for N_2 at $R = 2.068$ a.u. (experimental R_e) given by atomic STF SCF set+five 3d, five 4f, and one 5g is −108.9937 a.u. which is lower than that of Cade et al. (−108.9928 a.u.) [16] and that of Ermler and McLean (−108.9930 a.u.) [17]. It is close to the TE of NHF given by Christiansen and McCullough (−108.9939 a.u.) [18];

2) TE for P_2 at $R = 3.4978$ a.u. (calculated R_e of [19]) given by atomic STF SCF set+five 3d, five 4f, and one 5g is −681.50176 which is a little lower than that of Mulliken and Liu (−681.50039 a.u.)[19]. It is expected that the value given in the present work is as close to the HF limit as that for N_2. The details on the molecular calculations on N_2 and P_2 will be given elsewhere [15].

4. Conclusions

The atomic STF HF wavefunctions from B to Ca have been investigated. The size of the STF sets generated are (5s5p), (9s5p), (9s8p), and (12s8p) for B to Ne, Na to Mg, Al to Ar, and K to Ca, respectively. The differences in the total energies (TE's) between the numerical HF(NHF) and present calculations are less than 4×10^{-6} from B to F and less than 1×10^{-5} from Ne to Ca. These atomic wavefunctions are considered to provide standard basis sets for benchmark moleclar HF calculations. Similar atomic STF HF wavefunctions for transition metal atoms have been elsewhere [20].

Using the STF's for the atomic HF wavefunctions, we have performed molecular SCF calculations on N_2 and P_2. A large number of the polarization functions is required for reaching the HF limit.

The programs used were 'ALCHEMY'[21] and 'ATOM SCF' [22] where the open shell SCF method proposed by Roothaan and Bagus [1] is employed.

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