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Even-tempered Roothaan–Hartree–Fock wave functions for the third- and fourth-row atoms

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Summary. Roothaan–Hartree–Fock wave functions composed of 12s8p6d, 12s10p6d, and 12s10p8d even-tempered (ET) Slater-type functions (STFs), respectively, are reported for the atoms K–Zn, Ga–Kr, and Rb–Xe in their ground state. Despite the limited variational freedom in the ET method, the resultant atomic energies are found to compare well with fully-optimized wave functions of similar sizes. In particular, the present ET results reproduce almost completely the fully-optimized Sekiya–Tatewaki energies with the same basis set size for the atoms K–Zn. All the present energies are also lower than the Clementi–Roetti ones with slightly smaller but fully-optimized basis sets. A generalized even-tempered scheme is suggested and shown to give good results for Xe.

Key words: Even-tempered wave functions – Slater-type functions – Third- and fourth-row atoms

1 Introduction

Since the introduction of the analytical expansion or Roothaan–Hartree–Fock (RHF) method [1] in the Hartree–Fock (HF) theory, many atomic RHF wave functions have been generated using either Slater-type functions (STFs) or Gaussian-type functions (GTFs). Earlier elaborate work using STFs includes the RHF wave functions of Clementi [2], Bagus, Gilbert, and Roothaan [3], Huzinaga [4], and Raffenetti and Ruedenberg [5, 6]. In the first three of these efforts [2–4], the nonlinear parameters (i.e., STF exponents) were independently optimized. However, Raffenetti used the even-tempered (ET) representation of Ruedenberg, Raffenetti, and Bardo [7] in which the unnormalized radial parts of the STFs are given by $r^l \exp(-\zeta r)$ for all basis functions with the angular momentum quantum number l, and the exponents ζ for all the STFs corresponding to each l are given by a geometric sequence defined by two nonlinear parameters α and β.

The most extensive compilation of fully-optimized RHF wave functions is due to Clementi and Roetti [8]. Their RHF wave functions are widely considered to have near HF accuracy. They have been used extensively; for example, their work [8] received more than a thousand citations [9] in the first ten years after its publication. However, the insufficient accuracy of the Clementi–Roetti wave functions, compared to the numerical HF (NHF) results [10], has been pointed out often [11–16]. Improved STF-RHF wave functions were reported by Tatewaki and Sekiya [12–14] and Bunge et al. [15]. These authors made some effort to adopt optimal STF principal quantum numbers $\{n\}$ in addition to optimizing the exponents $\{\zeta\}$. The importance of the choice of $\{n\}$ has been demonstrated recently for He–Xe within the single-zeta [17] and double-zeta [18] approximations.

However, the apparent lack of regularities [17, 18] in the optimal $\{n\}$ makes it difficult to extend such an optimized basis set by adding more diffuse or tight basis functions that may be required for the description of some property other than the energy. On the other hand, there is no ambiguity in extending an ET basis set that uses only functions with the lowest value of n; one simply extends the geometric sequence of exponents. Thus, it is very useful to find ET basis sets that lead to energies comparable to those obtained from fully-optimized basis sets of similar size. There is evidence that this is possible. Ruedenberg and coworkers [5, 6, 19–22] showed that the HF limit can be achieved by the analytical expansion method using systematically large ET functions. The practical utility of the ET method was also supported by Huzinaga's [23] and Tatewaki's [24] findings that accurate atomic energies are obtained for the first- and second-row atoms by the use of a relatively small number of 1s and 2p STFs.

In this paper, we report RHF wave functions for the third- and fourth-row atoms in their ground state using even-tempered STF basis set of size comparable to fully-optimized ones. In the next section, the compuational method is described. In Sect. 3, the details of our wave functions are given. All our energies are closer to the NHF values than the famous Clementi–Roetti ones which were based upon slightly smaller STF sets. For the atoms K–Zn, the present results compare well with the fully-optimized results of Sekiya and Tatewaki [14], and Bunge et al. [15] and are satisfactory approximations to the NHF wave functions. In Sect. 4, we describe a generalized even-tempered scheme which is shown to give favorable results for Xe. Hartree atomic units are used throughout this paper.

2 Computational method

All the present RHF calculations were performed with a modified and corrected version [25] of Pitzer's implementation [26] of the Roothaan–Bagus procedure [1].

In the ET method [5–7, 19–22], the STF exponents $\{\zeta_i\}$ for each symmetry are specified by the two parameters α and β through the relationship:

$$\zeta_i = \alpha\beta^i, \qquad (i = 1, 2, \ldots, M_l)$$

where M_l is the number of basis STFs for the symmetry l ($=$ s, p, d, . . .). Thus only six nonlinear parameters are required for the third- and fourth-row atoms except for K and Ca which need only four. These nonlinear parameters were variationally optimized with Powell's conjugate directions method [27].

3 Results and discussion

The variational optimization of the tempering parameters $\{\alpha, \beta\}$ was performed for the atoms K–Zn with a 12s8p6d STF set, for Ga–Kr with a 12s10p6d STF set, and for Rb–Xe with a 12s10p8d STF set.

Table 1 presents a comparison of the total energies of our ET wave functions with those from fully-optimized wave functions [14, 8, 15] and NHF functions [10, 15]. We have the following observations about Table 1:

(i) For the atoms K–Zn, the present ET energies agree almost completely with those of the fully-optimized Sekiya–Tatewaki functions [14], though both calculations use exactly the same number of STFs. This implies that the Sekiya–Tatewaki functions can be further improved by the reoptimization of exponents. The results of Bunge et al. [15] support this statement since they obtained the same or better energies with a smaller basis set.

(ii) All our ET energies are lower than the Clementi–Roetti values [8]. Though we used slightly larger basis sets than Clementi and Roetti, this result is surprising since the Clementi–Roetti wave functions have been regarded as having near HF quality for a long time. The remarkable difference in the number of nonlinear parameters should be noted. In Xe, for example, our ET function has only 6 nonlinear parameters whereas the Clementi–Roetti function has 25.

(iii) As well as ζ-optimization, Bunge et al. [15] made a careful choice of $\{n\}$ and their energies coincide with the NHF values for almost all atoms. Except for the third-row atoms, our ET energies are worse than theirs. If we compare the number of STFs with Bunge et al. for K–Zn, where the total energies from the two calculations coincide, we see that our ET set contains one extra STF of each symmetry. This is in agreement with Feller and Davidson's observation [28] that the energy penalty to the ET method is about one STF in the carbon atom. Thus it is clear that our ET energies for the fourth-row atoms are worse than those of Bunge et al. in the third decimal place, because we used a smaller number of STFs. We think the present results are satisfactory given their basis size. However, a few more STFs are required to reproduce the NHF energies for the fourth-row atoms with the ET method.

Table 2 lists the values of the tempering parameters α and β. Adequate convergence of our optimization of these parameters is supported by the fact that the virial ratio did not deviate from its exact value (-2) by more than 1×10^{-7} in any of the present calculations. We have also verified that these parameters are smooth functions of the atomic number Z, except when the electronic configurations deviate from the simple aufbau pattern.

A detailed example of the present ET wave functions is given in Table 3 for the Fe atom, which occupies the central position of the third row in the periodic table. The ET orbital energies do not differ from the corresponding NHF values [10] by more than 5×10^{-5} a.u. and the near HF quality of the ET function is seen. The same is true for K–Zn.

4 Generalized even-tempered scheme

One may wonder whether the present results can be improved within the framework of the ET method without adding any STFs. We have found a simple

Table 1. Comparison of the atomic total energies (sign reversed) in a.u.

Z	Atom	Present ET		Sekiya–Tatewaki		Clementi–Roetti		Bunge et al.		NHF
		No. STFs	Energy	No. STFs	Energy	No. STFs	Energy	No. STFs	Energy	
19	K (^{2}S)	12s8p	599.16470	12s8p	599.16478	11s6p	599.16453	11s7p	599.16478	599.16479
20	Ca (^{1}S)	12s8p	676.75811	12s8p	676.75817	11s6p	676.75803	11s7p	676.75818	676.75819
21	Sc (^{2}D)	12s8p6d	759.73563	12s8p6d	759.73570	11s6p5d	759.73552	11s7p5d	759.73571	759.73572
22	Ti (^{3}F)	12s8p6d	848.40591	12s8p6d	848.40598	11s6p5d	848.40575	11s7p5d	848.40599	848.40600
23	V (^{4}F)	12s8p6d	942.88425	12s8p6d	942.88432	11s6p5d	942.88420	11s7p5d	942.88433	942.88434
24	Cr (^{7}S)	12s8p6d	1043.3563	12s8p6d	1043.3564	11s6p5d	1043.3552	11s7p5d	1043.3564	1043.3564
25	Mn (^{6}S)	12s8p6d	1149.8662	12s8p6d	1149.8662	11s6p5d	1149.8657	11s7p5d	1149.8662	1149.8663
26	Fe (^{5}D)	12s8p6d	1262.4436	12s8p6d	1262.4436	11s6p5d	1262.4432	11s7p5d	1262.4437	1262.4437
27	Co (^{4}F)	12s8p6d	1381.4145	12s8p6d	1381.4145	11s6p5d	1381.4142	11s7p5d	1381.4145	1381.4146
28	Ni (^{3}F)	12s8p6d	1506.8708	12s8p6d	1506.8709	11s6p5d	1506.8705	11s7p5d	1506.8709	1506.8709
29	Cu (^{2}S)	12s8p6d	1638.9636	12s8p6d	1638.9637	11s6p5d	1638.9628	11s7p5d	1638.9637	1638.9637
30	Zn (^{1}S)	12s8p6d	1777.8480	12s8p6d	1777.8481	11s6p5d	1777.8477	11s7p5d	1777.8481	1777.8481
31	Ga (^{2}P)	12s10p6d	1923.2608			10s9p5d	1923.2604	11s10p5d	1923.2610	1923.2610
32	Ge (^{3}P)	12s10p6d	2075.3595			10s9p5d	2075.3591	11s10p5d	2075.3597	2075.3597
33	As (^{4}S)	12s10p6d	2234.2385			10s9p5d	2234.2382	11s10p5d	2234.2386	2234.2387
34	Se (^{3}P)	12s10p6d	2399.8674			10s9p5d	2399.8658	11s10p5d	2399.8676	2399.8676
35	Br (^{2}P)	12s10p6d	2572.4412			10s9p5d	2572.4408	11s10p5d	2572.4413	2572.4413
36	Kr (^{1}S)	12s10p6d	2752.0548			10s9p5d	2752.0546	11s10p5d	2752.0550	2752.0550
37	Rb (^{2}S)	12s10p8d	2938.3553			11s7p3d	2938.3470	13s10p5d	2938.3574	2938.3575
38	Sr (^{1}S)	12s10p8d	3131.5439			11s7p3d	3131.5379	13s10p5d	3131.5457	3131.5457
39	Y (^{2}D)	12s10p8d	3331.6824			11s7p5d	3331.6712	13s10p8d	3331.6842	3331.6842
40	Zr (^{3}F)	12s10p8d	3538.9932			11s7p5d	3538.9821	13s10p8d	3538.9951	3538.9951
41	Nb (^{6}D)	12s10p8d	3753.5959			11s7p5d	3753.5845	13s10p8d	3753.5977	3753.5977
42	Mo (^{7}S)	12s10p8d	3975.5475			11s7p5d	3975.5338	13s10p8d	3975.5495	3975.5495
43	Tc (^{6}S)	12s10p8d	4204.7863			11s7p5d	4204.7753	13s10p8d	4204.7887	4204.7887
44	Ru (^{5}F)	12s10p8d	4441.5368			11s7p5d	4441.5264	13s10p8d	4441.5395	4441.5395
45	Rh (^{4}F)	12s10p8d	4685.8786			11s7p5d		13s10p8d	4685.8817	4685.8817
46	Pd (^{1}S)	12s10p8d	4937.9203			9s7p5d	4937.9071	13s10p8d	4937.9210	4937.9210
47	Ag (^{2}S)	12s10p8d	5197.6946			11s7p5d	5197.6852	13s10p8d	5197.6985	5197.6985
48	Cd (^{1}S)	12s10p8d	5465.1296			11s7p5d	5465.0722	13s10p8d	5465.1331	5465.1331
49	In (^{2}P)	12s10p8d	5740.1648			11s9p5d	5740.1570	13s12p8d	5740.1691	5740.1692
50	Sn (^{3}P)	12s10p8d	6022.9281			11s9p5d	6022.9220	13s12p8d	6022.9317	6022.9317
51	Sb (^{4}S)	12s10p8d	6313.4822			11s9p5d	6313.4755	13s12p8d	6313.4853	6313.4853
52	Te (^{3}P)	12s10p8d	6611.7812			11s9p5d	6611.7748	13s12p8d	6611.7840	6611.7841
53	I (^{2}P)	12s10p8d	6917.9782			11s9p5d	6917.9727	13s12p8d	6917.9809	6917.9809
54	Xe (^{1}S)	12s10p8d	7232.1359			11s9p5d	7232.1302	13s12p8d	7232.1383	7232.1384

Table 2. Parameters of the even-tempered wave functions

Z	Atom	s		p		d	
		α	β	α	β	α	β
19	K (^{2}S)	0.323156	1.500168	1.085373	1.412995		
20	Ca (^{1}S)	0.386367	1.481109	1.091284	1.427859		
21	Sc (^{2}D)	0.433048	1.414489	1.206324	1.420436	0.653988	1.599321
22	Ti (^{3}F)	0.444283	1.418205	1.319584	1.412493	0.747917	1.580641
23	V (^{4}F)	0.454140	1.422116	1.424874	1.407294	0.809027	1.577057
24	Cr (^{7}S)	0.441656	1.432744	1.484347	1.413282	0.690256	1.642520
25	Mn (^{6}S)	0.471853	1.429669	1.620072	1.401390	0.915593	1.576429
26	Fe (^{5}D)	0.483640	1.432193	1.705249	1.403325	0.926453	1.591982
27	Co (^{4}F)	0.494611	1.434749	1.790105	1.404884	0.951912	1.602116
28	Ni (^{3}F)	0.505546	1.437127	1.873375	1.406744	0.979097	1.611376
29	Cu (^{2}S)	0.473332	1.451328	1.816616	1.384481	0.827552	1.688536
30	Zn (^{1}S)	0.526862	1.441530	1.988673	1.377547	1.041109	1.626022
31	Ga (^{2}P)	0.626313	1.422503	0.489039	1.503293	1.250979	1.580672
32	Ge (^{3}P)	0.718485	1.408212	0.581931	1.478153	1.391589	1.566362
33	As (^{4}S)	0.809263	1.396284	0.671720	1.458912	1.558204	1.552310
34	Se (^{3}P)	0.889055	1.387678	0.709062	1.455770	1.752082	1.535982
35	Br (^{2}P)	0.963935	1.380802	0.764697	1.448794	1.944485	1.524544
36	Kr (^{1}S)	1.049276	1.373751	0.834230	1.439216	2.127623	1.518821
37	Rb (^{2}S)	0.340918	1.527497	1.006430	1.412036	0.425759	1.691187
38	Sr (^{1}S)	0.393940	1.511817	0.934467	1.430821	0.474442	1.672810
39	Y (^{2}D)	0.422139	1.506049	1.026911	1.419959	0.529066	1.653825
40	Zr (^{3}F)	0.440533	1.503631	1.100140	1.413366	0.583895	1.636895
41	Nb (^{6}D)	0.475851	1.496666	1.176644	1.406577	0.643000	1.620231
42	Mo (^{7}S)	0.489557	1.495912	1.261091	1.399586	0.716652	1.597448
43	Tc (^{6}S)	0.477542	1.501934	1.322453	1.396620	0.907124	1.514435
44	Ru (^{5}F)	0.492628	1.500668	1.400252	1.391417	0.822341	1.574196
45	Rh (^{4}F)	0.490705	1.503923	1.475139	1.387229	0.880908	1.559883
46	Pd (^{1}S)	1.306916	1.379291	1.513970	1.387684	0.704067	1.534819
47	Ag (^{2}S)	0.484166	1.511185	1.634369	1.378923	0.937174	1.487945
48	Cd (^{1}S)	0.520962	1.504179	1.711569	1.375711	1.154935	1.491807
49	In (^{2}P)	0.620819	1.484194	0.499604	1.520617	1.309980	1.465562
50	Sn (^{3}P)	0.699430	1.471779	0.546553	1.508798	1.434752	1.451910
51	Sb (^{4}S)	0.768925	1.462490	0.590590	1.499171	1.541278	1.444441
52	Te (^{3}P)	0.833152	1.454979	0.616791	1.495490	1.641393	1.439100
53	I (^{2}P)	0.893343	1.448702	0.650000	1.490162	1.733196	1.435872
54	Xe (^{1}S)	0.951017	1.443253	0.686055	1.484517	1.820085	1.433470

modification that may produce nontrivial improvements for the fourth-row atoms. The idea is to use two even-tempered sequences with different principal quantum numbers: 1s and 2s, 2p and 3p, and 3d and 4d STFs for the s, p, and d symmetries. For example, a set of 1s type STFs, $\exp(-\zeta r)$, with the ζ in a geometric sequence and a set of 2s STFs, $r\exp(-\zeta' r)$, with the ζ' in a *different* geometric sequence form the s-part of the basis set. Thus, the number of nonlinear parameters is exactly twice that of the original ET method. A preliminary examination of this scheme was made for Xe. Tables 4 and 5 display the conventional ET and generalized ET wave functions for Xe in a basis set of 12s10p8d STFs. The error with respect to the

Table 3. Even-tempered wave function for the Fe atom

IRON K(2)L(8)3S(2)3P(6)4S(2)3D(6), 5D

E = −1262.44357760
T = 1262.44357780 V = −2524.88715540 V/T = −2.00000000
Orbital energies and expansion coefficients

S		1S	2S	3S	4S
BASIS/ORB.ENERGY		−261.3733781	−31.9354695	−4.1693918	−0.2581549
1S	0.692666	0.0004055	−0.0023350	−0.0098949	2.1369588
1S	0.992031	−0.0022897	0.0134027	0.0499342	−1.1774061
1S	1.420781	0.0068235	−0.0409618	−0.1233153	0.3405459
1S	2.034832	−0.0144809	0.0906632	0.2011115	−1.0817492
1S	2.914273	0.0247491	−0.1636000	1.7140601	0.4258904
1S	4.173802	−0.0365136	0.2815595	0.4614936	−0.4991230
1S	5.977692	0.0473860	−0.4060962	−2.3067162	0.7587552
1S	8.561210	−0.0551136	2.6444617	−0.2309296	−0.0556254
1S	12.261307	0.0599210	−1.2648598	0.7489488	−0.1448601
1S	17.560561	−0.0205375	−0.5321771	0.0504810	−0.0115755
1S	25.150118	0.9430599	−0.0576182	0.0471938	−0.0098701
1S	36.019829	0.0509094	−0.0037891	−0.0027918	0.0005951

P		2P	3P
BASIS/ORB.ENERGY		−27.4136681	−2.7421626
2P	2.393018	0.0037274	0.2518936
2P	3.358182	− 0.0159807	0.7487926
2P	4.712621	0.0455896	0.2849138
2P	6.613339	− 0.0501728	−0.1617175
2P	9.280664	0.6779521	−0.4340381
2P	13.023787	0.3167296	−0.0265901
2P	18.276607	0.0421142	−0.0340968
2P	25.648019	0.0073560	0.0007164

D		3D
BASIS/ORB.ENERGY		−0.6468586
3D	1.474896	0.1261427
3D	2.348007	0.3486678
3D	3.737984	0.3836182
3D	5.950801	0.2582315
3D	9.473566	0.0400456
3D	15.081741	0.0056755

numerical HF limit is reduced from 2.5 to 1.0 millihartrees by changing from the conventional to the generalized ET scheme. The use of two *n*'s seems to reduce the numerical linear dependence resulting in an improved atomic energy.

5 Summarizing remarks

In summary, we have reported accurate ET-RHF wave functions for the atoms K–Xe. Among the present ET functions, those for K–Zn described with 12s8p6d STF sets have quality close to the NHF functions. The slight increase in size of an ET basis over a fully-optimized one is more than compensated by a marked

Table 4. Conventional even-tempered wave function for the Xe atom

XENON K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(6), IS

E = – 7232.13585050
T = 7232.13585186 V = – 14464.27170236 V/T = – 2.00000000
Orbital energies and expansion coefficients

S		1S	2S	3S	4S	5S
BASIS/ORB.ENERGY		– 1224.3951860	– 189.3393911	– 40.1748522	– 7.8554279	– 0.9440251
1S	1.372558	– 0.0000885	– 0.0115554	– 0.0234280	– 0.0212616	3.1079091
1S	1.980949	0.0004885	0.0635889	0.1305101	0.1396986	– 2.0416369
1S	2.859011	– 0.0014323	– 0.1846242	– 0.3947839	– 0.3973455	– 0.8735901
1S	4.126276	0.0030065	0.3826031	0.8936627	5.3905864	– 1.8519813
1S	5.955262	– 0.0050900	– 0.6460441	– 1.7364365	– 5.5846382	3.1790136
1S	8.594951	0.0075863	0.9584605	5.8612449	– 2.1921480	– 0.0014464
1S	12.404692	– 0.0107848	– 1.3500553	– 4.5446812	4.3651847	– 1.3039577
1S	17.903112	0.0144935	3.1921481	– 1.2195399	– 0.8097296	0.1891482
1S	25.838726	– 0.0204878	– 0.9648946	1.4993249	– 0.2564800	0.1474907
1S	37.291825	0.0624047	– 0.9548934	0.0624855	– 0.1530115	0.0308365
1S	53.821549	0.9363043	0.0600756	0.0243014	0.0203013	– 0.0013901
1S	77.678128	0.0159241	– 0.0108407	– 0.0015572	– 0.0031524	0.0003493

P		2P	3P	4P	5P
BASIS/ORB.ENERGY		– 177.7816670	– 35.2208344	– 6.0074382	– 0.4567536
2P	1..018461	– 0.0002543	– 0.0008474	0.0023317	0.5067037
2P	1.511923	0.0011140	0.0040278	– 0.0035841	0.8239016
2P	2.244475	– 0.0026621	– 0.0111322	– 0.0120617	– 0.0354575
2P	3.331961	0.0046520	0.0244739	0.4102889	– 0.6728875
2P	4.946353	– 0.0069651	– 0.0479906	1.7574325	– 0.4144580
2P	7.342944	0.0090371	0.2300553	– 1.5744823	0.5179530
2P	10.900726	– 0.0148860	1.5731912	– 0.5662604	0.1877832
2P	16.182313	0.0943007	– 0.8584820	0.4908815	– 0.1669586
2P	24.022919	0.8244323	– 0.3666768	0.1417159	– 0.0395340
2P	35.662431	0.1070062	– 0.0288847	0.0134445	– 0.0045536

D		3D	4D
BASIS/ORB.ENERGY		– 26.1182786	– 2.7770778
3D	2.609036	0.0010448	0.0907797
3D	3.739974	– 0.0045696	0.5096281
3D	5.361139	0.0098235	0.5935054
3D	7.685030	0.0527882	– 0.0452980
3D	11.016256	0.6044724	– 0.3597518
3D	15.791467	0.3207948	– 0.1125893
3D	22.636587	0.0628014	– 0.0332165
3D	32.448858	0.0040749	– 0.0002810

reduction in the number of nonlinear parameters to be optimized and ease of extension. We hope the ET wave functions reported in this paper will be of some use in future atomic and molecular studies. Detailed tables of these wave functions are available, preferably via Internet upon request to AJIT@UNB.CA, or by post to TK or AJT. The generalized ET will be explored further.

Table 5. Generalized even-tempered wave function for the Xe atom

XENON K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(6), IS

E = – 7232.13735779
T = 7232.13737294 V = – 14464.27473074 V/T = – 2.00000000
Orbital energies and expansion coefficients

S		1S	2S	3S	4S	5S
BASIS/ORB.ENERGY		– 1224.3972289	– 189.3396696	– 40.1753255	– 7.8557437	– 0.9441867
1S	2.636182	– 0.0010485	0.0974930	– 0.3483920	– 0.8619892	3.0172120
1S	4.891944	– 0.0028091	0.0629619	– 0.1457771	6.4102194	– 3.6919876
1S	9.077947	– 0.0127133	0.1849803	3.2952954	– 3.1080046	1.1835238
1S	16.845884	– 0.0977944	2.7915104	– 2.0064296	0.5534352	– 0.1571512
1S	31.260792	0.8190088	– 1.8314808	0.6147637	– 0.2565749	0.0856158
1S	58.010436	0.5813945	– 0.0153418	0.0029879	– 0.0002676	– 0.0006425
2S	0.695142	– 0.0000006	0.0002290	– 0.0008729	– 0.0007489	0.0190425
2S	1.550611	0.0000107	– 0.0019353	0.0071189	0.0109404	1.2567475
2S	3.458851	0.0009102	– 0.0732945	0.2586757	0.9316310	– 2.6245937
2S	7.715444	0.0050241	– 0.1223226	0.3264329	– 4.3014362	1.8108616
2S	17.210364	0.0438690	– 0.7388776	– 1.5672781	0.7643513	– 0.2851486
2S	38.390093	– 0.3774166	0.0631672	– 0.0185959	0.0102266	– 0.0059338

P		2P	3P	4P	5P
BASIS/ORB.ENERGY		– 177.7821036	– 35.2213832	– 6.0077954	– 0.4570459
2P	2.114683	0.0069415	0.0272005	– 0.0838584	3.4171156
2P	4.255573	0.0136328	0.0560894	1.4724400	– 2.6429294
2P	8.563885	0.0314438	0.6307173	– 1.5145784	0.9059817
2P	17.233901	0.2462966	– 0.3939708	0.4052952	– 0.1644379
2P	34.681378	0.4147141	– 0.1650624	0.0626490	– 0.0172437
3P	1.266148	– 0.0001907	– 0.0007631	0.0026851	0.5423893
3P	2.775040	– 0.0070366	– 0.0275603	0.1017780	– 2.1483695
3P	6.082103	– 0.0175935	– 0.0700765	0.1663494	0.8053417
3P	13.330253	– 0.0494440	0.6795408	0.0114631	– 0.0566308
3P	29.216150	0.4059361	– 0.1837928	0.0658678	– 0.0162473

D		3D	4D
BASIS/ORB.ENERGY		– 26.1185065	– 2.7773615
3D	2.798988	– 0.0004976	0.1747423
3D	6.132540	0.0156914	0.6184946
3D	13.436301	0.7092478	– 0.3470345
3D	29.438730	0.0414469	– 0.0170266
4D	2.082013	0.0001125	0.0024516
4D	4.751155	– 0.0002484	0.4904857
4D	10.842140	0.2332083	– 0.2327102
4D	24.741773	0.0719452	– 0.0313704

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