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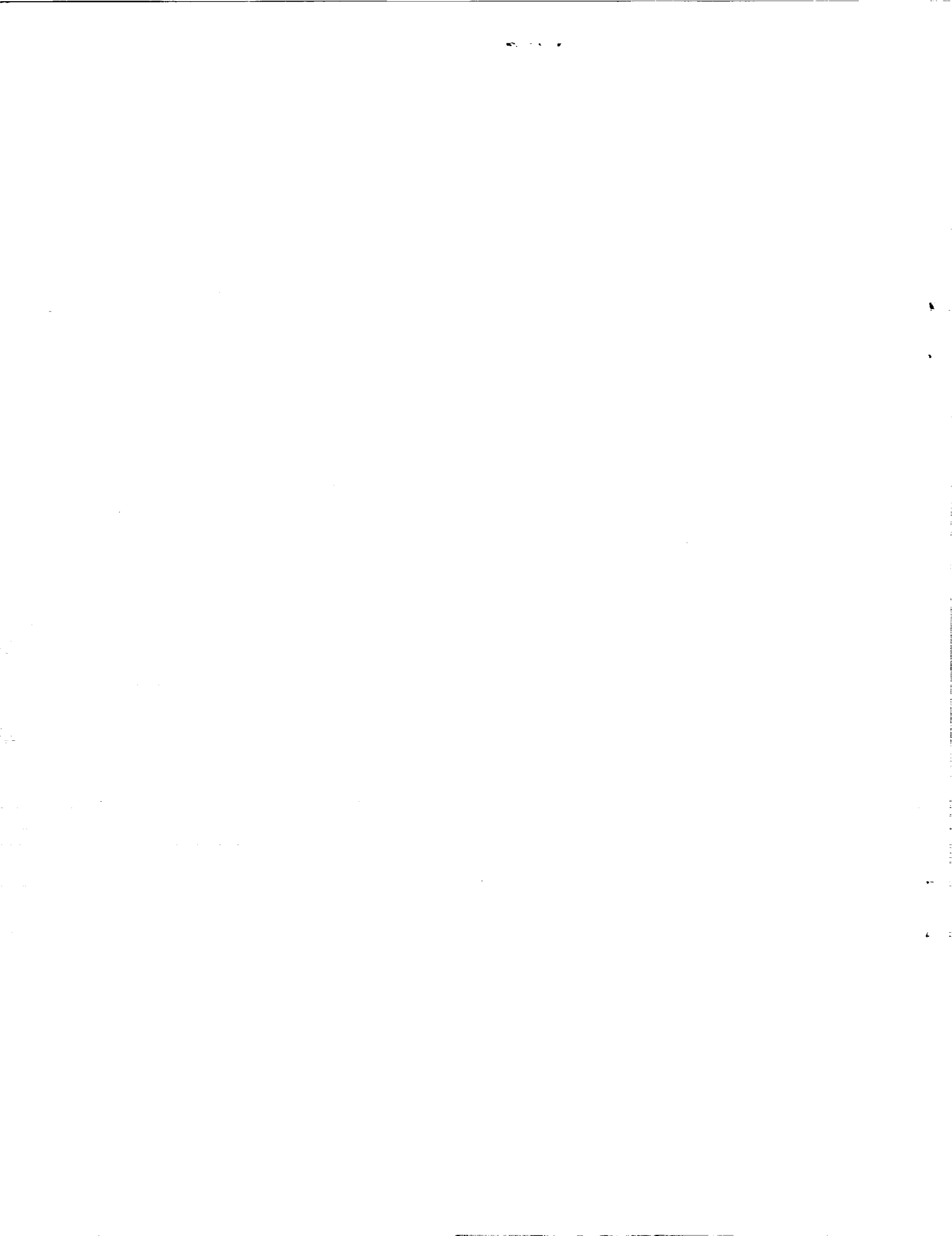
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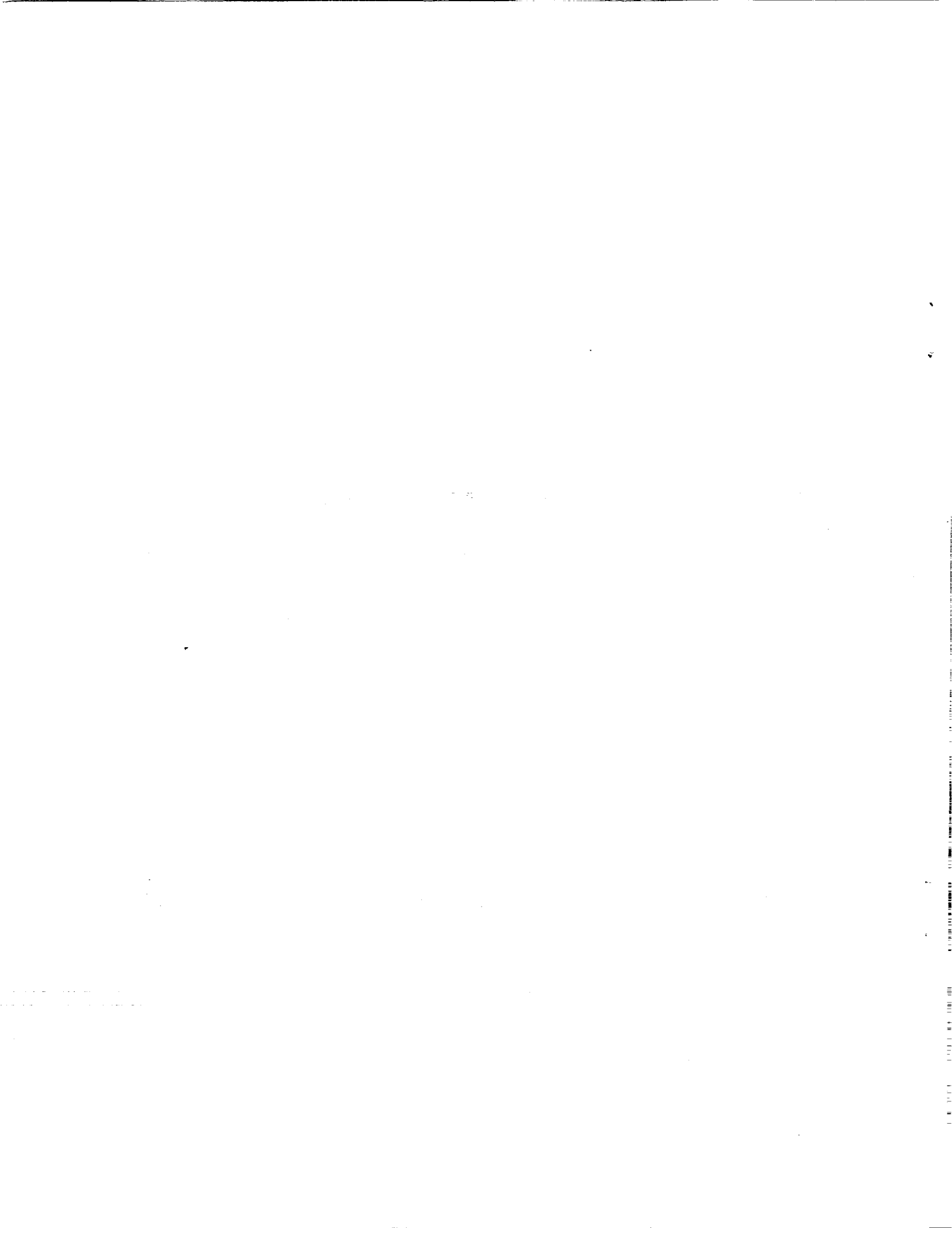
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HIGH-QUALITY GAUSSIAN BASIS SETS FOR FOURTH-ROW ATOMS

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SUMMARY

Energy-optimized Gaussian basis sets of triple-zeta quality for the atoms Rb—Xe have been derived. Two series of basis sets are developed: (24s 16p 10d) and (26s 16p 10d) sets which we expand to 13 *d* and 19 *p* functions as the 4*d* and 5*p* shells become occupied. For the atoms lighter than Cd, the (24s 16p 10d) sets with triple-zeta valence distributions are higher in energy than the corresponding double-zeta distribution. To ensure a triple-zeta distribution and a global energy minimum, the (26s 16p 10d) sets were derived. Total atomic energies from the largest basis sets are between 198 and 284 μE_H above the numerical Hartree-Fock energies.

INTRODUCTION

Modern computational chemistry is to a large extent based on the use of finite basis sets of Gaussian-type orbitals (GTOs) for analytic expansion of one-particle functions. First introduced in quantum chemistry by Boys in 1950 (ref. 1), GTOs permit rapid evaluation of multicenter two-electron integrals, and for calculations on polyatomic molecules there is presently no practical alternative.

The chief disadvantage of GTO basis sets is that the functions give a poor representation of the region close to the atomic nucleus; thus, for very accurate work a large number of basis functions are needed. Integral evaluation time was a limiting factor in earlier work, but the availability of more powerful computers and the development of efficient integral evaluation algorithms have reduced this limitation significantly. Today, in highly accurate work with an extensive treatment of electron correlation, the integral evaluation usually accounts for a relatively small fraction of the total computational effort. In addition, general contraction schemes, such as the recently developed atomic natural orbital (ANO) method (ref. 2), explicitly intended for use in correlated calculations, have eliminated much of the burden of handling large basis sets beyond the integral evaluation stage. At the same time, state-of-the-art calculations have reached the point where the lack of high-quality basis sets can be an obstacle for accurate studies (refs. 3-6).

For some time we have been involved in the development of high-quality energy-optimized GTO basis sets (refs. 7-11). In this work we extend these efforts to include sets of triple zeta

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(TZ) quality — representing the main amplitude of each atomic orbital by at least three primitive GTO functions — for the fourth-row elements. Basis sets for all of these elements or for groups of them have been derived previously by Faegri and Biran (ref. 11), Huzinaga (ref. 12), Hyla-Krispin et al. (ref. 13), and Gropen (ref. 14), and also special sets such as the MINI and MIDI (ref. 15) and well-tempered sets (ref. 16) exist. However, since none of these are of TZ quality, the sets presented here are significantly more accurate. Although relativistic effects become somewhat important for this row, they can to a large extent be accounted for through first-order perturbation theory. Thus the basis sets presented in this work will be principally useful for nonrelativistic calculations in which it is desirable to minimize the inaccuracies arising from the finite-basis approximation—see, for example, reference 17. In addition, these basis sets, supplemented with additional compact functions, should be useful for high-quality relativistic calculations (ref. 18).

This report work has been summarized in reference 19, and the basis sets are available from the Quantum Chemistry Program Exchange (QCPE, Bloomington, Indiana 47401).

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RESULTS AND DISCUSSION

The details of our computational method and the strategies followed in energy optimizations of these basis sets have been described previously (refs. 7-9). We have carried out pilot calculations on Ag and Xe to determine the size of basis set needed to obtain an energy-balanced triple-zeta valence description. Unfortunately, because of the size of the basis required for a TZ valence distributions, we are faced with a problem of multiple energy minima. This has been discussed for the first-row transition metal atoms (ref. 8) and manifests itself in two close-lying minima on the energy surface, each corresponding to a different distribution of orbital exponents. For Ag it was possible to find a $(23s\ 15p\ 12d)$ basis set which had a TZ valence description, but this size of basis set did not support a TZ minimum for the elements lighter than Rh. Increasing the size to $(24s\ 16p\ 13d)$, corresponding to $(24s\ 16p\ 10d)$ for elements without occupied $4d$ orbitals, and $(24s\ 19p\ 13d)$ for elements with occupied $5p$ orbitals, we are able to locate TZ minima for all atoms of the row except Rb, Sr, and Y. However, even for basis sets of this size, more energy is gained by improving the $4s$ description than by providing a TZ $5s$, and therefore distributions yielding a double zeta (DZ) $5s$ are lower in energy for the elements lighter than Cd.

To provide basis sets that ensure a TZ distribution and a global energy minimum, we have also derived $(26s\ 16p\ 10d)$ sets supplemented by additional basis functions as the $4d$ and $5p$ shells become occupied. Thus, our largest set for Y is $(26s\ 16p\ 13d)$, and the corresponding Xe set is $(26s\ 19p\ 13d)$. For these sets the TZ distribution represents a stable, single minimum, with no competing DZ minimum nearby.

The problem with stabilizing the TZ distribution also influences the choice of atomic state used in the optimization of the basis sets. The states derived from the orbital occupations $5s^2 4d^n$, $5s^1 4d^{n+1}$, and $5s^0 4d^{n+2}$ are close in energy for the transition metal atoms of the

fourth row, and only Y, Zr, Tc, and Cd have a $5s^24d^n$ ground state configuration; Pd has $5s^04d^{n+2}$, and Nb, Mo, Ru, Rh, and Ag have $5s^14d^{n+1}$ ground states. For transition metal atoms, rather than using the ground states, we have chosen to use the lowest $5s^24d^n$ states for the orbital exponent optimizations, for this stabilizes the TZ distribution for the 5s shell — with more 5s electrons the contribution to the total electronic energy from this shell increases, making an optimal description of the 5s orbital important. Also, experience with calculations involving transition metal atoms has shown that the basis sets optimized for the lowest s^2d^n state, supplemented with suitable diffuse functions, yield a balanced description of the low-lying states (ref. 20), and provide a good starting point for molecular calculations where states derived from several of these occupations interact.

The energies obtained with the various basis sets are listed in table I, where we also give a comparison with the numerical Hartree-Fock (NHF) results. All energies calculated with the basis sets containing 24 s functions are within $400 \mu E_H$ of the numerical results, and the 26 s sets have a maximum deviation of $284 \mu E_H$ (for Cd) and, for most sets, are within $250 \mu E_H$ of the NHF results. The apparently discontinuous improvement in quality between Cd and In is due to the addition of three p functions which not only describe the 5p shell, but also improve the description of the inner p shells. Supplementary functions were also optimized to describe Rb (2P), Sr (3P), and I^- (1S). However, the energy improvement over employing even-tempered diffuse functions (ratio of 2.5) is insignificant. For the transition metal atoms, experience has shown that adding an even-tempered d function and three even-tempered p functions is adequate (refs. 10 and 19). The basis sets, the orbital exponents, and eigenvectors for the basis sets are given in tables II to LXVII.

CONCLUSIONS

Energy-optimized high-quality GTO basis sets have been presented for the fourth-row atoms, Rb to Xe. The largest sets have a TZ valence distribution and are within $284 \mu E_H$ of the NHF energy.

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Table I. Atomic energies for fourth-row atoms from numerical Hartree-Fock (NHF) and finite basis (GTO) calculations in hartree units (E_H), and their difference (Δ) in μE_H . DZ (TZ) - double (triple) zeta for 5s shell.

Atom	NHF energy	Basis	GTO energy	Δ
Rb (2S)	-2938.357457	24,16,10 DZ	-0.357225	232
		26,16,10	-0.357254	203
Sr (1S)	-3131.545689	24,16,10 DZ	-0.545457	232
		26,16,10	-0.545491	198
Y (2D)	-3331.684169	24,16,13 DZ	-0.683920	249
		26,16,13	-0.683964	205
Zr (3F)	-3538.995065	24,16,13 DZ	-0.994805	260
		24,16,13 TZ	-0.994784	281
		26,16,13	-0.994855	210
Nb (4F)	-3753.552031	24,16,13 DZ	-0.551759	272
		24,16,13 TZ	-0.551742	289
		26,16,13	-0.551816	215
Mo (5D)	-3975.443320	24,16,13 DZ	-0.443036	284
		24,16,13 TZ	-0.443022	298
		26,16,13	-0.443098	222
Tc (6S)	-4204.788736	24,16,13 DZ	-0.788442	294
		24,16,13 TZ	-0.788431	305
		26,16,13	-0.788509	227
Ru (5D)	-4441.487348	24,16,13 DZ	-0.487032	316
		24,16,13 TZ	-0.487026	322
		26,16,13	-0.487105	243
Rh (4F)	-4685.801249	24,16,13 DZ	-0.800916	333
		24,16,13 TZ	-0.800914	335
		26,16,13	-0.800996	253
Pd (3F)	-4937.783027	24,16,13 DZ	-0.782677	350
		24,16,13 TZ	-0.782679	348
		26,16,13	-0.782764	263
Ag (2D)	-5197.517887	24,16,13 DZ	-0.517520	367
		24,16,13 TZ	-0.517526	361
		26,16,13	-0.517613	274
Cd (1S)	-5465.133142	24,16,13 DZ	-0.132758	384
		24,16,13 TZ	-0.132768	374
		26,16,13	-0.132858	284
In (2P)	-5740.169155	24,19,13 DZ	-0.168834	321
		24,19,13 TZ	-0.168848	307
		26,19,13	-0.168938	217
Sn (3P)	-6022.931695	24,19,13 TZ	-0.931397	298
		26,19,13	-0.931486	209
Sb (4S)	-6313.485321	24,19,13 TZ	-0.485029	292
		26,19,13	-0.485117	204
Te (3P)	-6611.784059	24,19,13 TZ	-0.783821	297
		26,19,13	-0.783850	209
I (2P)	-6917.980895	24,19,13 TZ	-0.980596	299
		26,19,13	-0.980685	210
Xe (1S)	-7232.138365	24,19,13 TZ	-0.138065	300
		26,19,13	-0.138154	211

Table II. Rb 2S ($24s16p10d$) basis set. Energy(E_H) = -2938.357225

Exponent	s space				
	1s	2s	3s	4s	5s
	-551.457280	-75.049293	-12.133146	-1.523512	-0.137848
33676620.	0.000002	-0.000001	0.000000	0.000000	0.000000
5043176.	0.000013	-0.000004	0.000002	-0.000001	0.000000
1147775.	0.000066	-0.000021	0.000008	-0.000003	0.000001
325140.5	0.000279	-0.000088	0.000036	-0.000012	0.000003
106090.9	0.001016	-0.000321	0.000130	-0.000044	0.000009
38307.63	0.003312	-0.001049	0.000425	-0.000144	0.000030
14944.27	0.009850	-0.003140	0.001273	-0.000430	0.000090
6200.050	0.026871	-0.008693	0.003532	-0.001196	0.000252
2705.265	0.066622	-0.022247	0.009074	-0.003064	0.000645
1230.926	0.145360	-0.051883	0.021358	-0.007248	0.001526
580.0102	0.260631	-0.106151	0.044455	-0.015062	0.003175
281.2328	0.334868	-0.175242	0.076118	-0.026100	0.005499
138.8341	0.239880	-0.177433	0.081796	-0.028003	0.005919
67.42336	0.059138	0.058405	-0.030505	0.010119	-0.002159
34.60051	-0.000245	0.481780	-0.324803	0.120902	-0.025660
17.75368	0.001592	0.492815	-0.482403	0.185501	-0.039747
8.897414	-0.000795	0.131668	0.014870	-0.005171	0.001223
4.394148	0.000356	0.004812	0.699537	-0.382949	0.085159
2.164604	-0.000195	0.001819	0.504523	-0.487077	0.116751
0.846716	0.000094	-0.000529	0.046811	0.257094	-0.079186
0.423673	-0.000053	0.000222	-0.006290	0.732544	-0.207295
0.192624	0.000017	-0.000091	0.002045	0.310395	-0.259416
0.033338	-0.000004	0.000017	-0.000296	0.004999	0.723839
0.014695	0.000002	-0.000008	0.000137	-0.001236	0.427067
p space			d space		
Exponent	2p	3p	4p	Exponent	3d
	-67.906170	-9.487641	-0.810034		-4.732236
32035.95	0.000055	-0.000023	0.000007	1096.370	0.000236
7583.905	0.000488	-0.000201	0.000060	330.8446	0.002251
2463.139	0.002814	-0.001163	0.000347	128.8062	0.012635
942.3746	0.012347	-0.005152	0.001542	56.84727	0.047548
399.8539	0.043336	-0.018378	0.005509	26.87133	0.129664
182.3892	0.120882	-0.053145	0.016022	13.26207	0.250659
87.54580	0.253719	-0.116912	0.035461	6.620098	0.338547
43.48637	0.363730	-0.179145	0.055039	3.291086	0.311974
22.08999	0.288507	-0.113541	0.032772	1.589852	0.158396
11.14450	0.092012	0.184923	-0.072448	0.688999	0.028360
5.551092	0.007079	0.479808	-0.190064		
2.751542	0.001286	0.396422	-0.186542		
1.304547	-0.000242	0.091705	0.114546		
0.614990	0.000149	0.001286	0.475033		
0.275799	-0.000066	0.001270	0.463882		
0.116148	0.000018	-0.000274	0.122916		

Table III. Rb 2S (26s16p10d) basis set. Energy(E_H) = -2938.357254

Exponent	s space				
	1s	2s	3s	4s	5s
	-551.457290	-75.049301	-12.133153	-1.523517	-0.137847
57550850.	0.000001	0.000000	0.000000	0.000000	0.000000
8615114.	0.000006	-0.000002	0.000001	0.000000	0.000000
1960347.	0.000034	-0.000011	0.000004	-0.000001	0.000000
555343.6	0.000143	-0.000045	0.000018	-0.000006	0.000001
181234.8	0.000521	-0.000164	0.000067	-0.000023	0.000005
65458.36	0.001701	-0.000538	0.000218	-0.000074	0.000015
25545.29	0.005086	-0.001615	0.000655	-0.000221	0.000047
10603.16	0.014059	-0.004499	0.001825	-0.000616	0.000130
4629.569	0.035894	-0.011714	0.004766	-0.001613	0.000339
2108.902	0.083346	-0.028263	0.011550	-0.003901	0.000822
995.7281	0.169277	-0.062188	0.025701	-0.008728	0.001836
484.6410	0.278616	-0.118973	0.050145	-0.017005	0.003589
241.8381	0.320417	-0.180461	0.079260	-0.027234	0.005728
122.3508	0.199309	-0.151544	0.070808	-0.024256	0.005153
59.93350	0.040418	0.123868	-0.066635	0.022925	-0.004926
31.42571	-0.000963	0.507498	-0.360434	0.135275	-0.028622
16.43267	0.001294	0.443008	-0.447177	0.172510	-0.037213
8.333295	-0.000667	0.105624	0.078471	-0.032132	0.007458
4.233272	0.000303	0.003253	0.693184	-0.387381	0.085640
2.134369	-0.000174	0.001818	0.475358	-0.468687	0.113831
0.877086	0.000093	-0.000584	0.048409	0.221237	-0.072258
0.449830	-0.000061	0.000293	-0.006815	0.703666	-0.187903
0.212610	0.000028	-0.000160	0.003007	0.364615	-0.262705
0.075589	-0.000012	0.000064	-0.000941	0.016826	-0.070644
0.035913	0.000007	-0.000036	0.000503	-0.001849	0.715670
0.015307	-0.000002	0.000009	-0.000131	0.000577	0.481470
	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	-67.906176	-9.487646	-0.810039		-4.732242
32052.83	0.000055	-0.000023	0.000007	1096.422	0.000236
7587.801	0.000488	-0.000201	0.000060	330.8525	0.002251
2464.371	0.002812	-0.001162	0.000347	128.8072	0.012635
942.8340	0.012337	-0.005148	0.001541	56.84694	0.047549
400.0438	0.043306	-0.018365	0.005505	26.87088	0.129668
182.4734	0.120813	-0.053114	0.016013	13.26184	0.250660
87.58571	0.253618	-0.116862	0.035446	6.620043	0.338542
43.50635	0.363690	-0.179119	0.055030	3.291083	0.311973
22.10053	0.288623	-0.113669	0.032819	1.589852	0.158396
11.15042	0.092127	0.184629	-0.072347	0.689000	0.028360
5.554370	0.007100	0.479647	-0.189970		
2.753327	0.001287	0.396656	-0.186671		
1.305694	-0.000242	0.091904	0.114104		
0.615472	0.000149	0.001310	0.474919		
0.275961	-0.000066	0.001268	0.464211		
0.116192	0.000018	-0.000273	0.123070		

Table IV. Sr 1S ($24s16p10d$) basis set. Energy(E_H) = -3131.545457

Exponent	s space				
	1s	2s	3s	4s	5s
	-583.687820	-80.390738	-13.474971	-1.896771	-0.178423
44174240.	0.000001	0.000000	0.000000	0.000000	0.000000
6544609.	0.000010	-0.000003	0.000001	0.000000	0.000000
1475561.	0.000052	-0.000016	0.000007	-0.000002	0.000001
414639.5	0.000221	-0.000070	0.000029	-0.000010	0.000003
134348.0	0.000814	-0.000258	0.000105	-0.000037	0.000010
48211.79	0.002677	-0.000849	0.000347	-0.000123	0.000032
18704.85	0.008030	-0.002563	0.001049	-0.000373	0.000096
7722.153	0.022150	-0.007152	0.002930	-0.001042	0.000269
3354.674	0.055791	-0.018535	0.007624	-0.002714	0.000699
1520.642	0.124994	-0.043915	0.018188	-0.006484	0.001675
714.3551	0.234608	-0.092614	0.038988	-0.013930	0.003587
345.8466	0.327929	-0.160799	0.069753	-0.025064	0.006490
171.4040	0.273073	-0.190253	0.087368	-0.031655	0.008139
85.89144	0.092150	-0.024550	0.011947	-0.004506	0.001269
42.86507	0.005516	0.396653	-0.250156	0.096094	-0.025250
22.00691	0.000924	0.545466	-0.500589	0.203751	-0.052996
11.26820	-0.000427	0.206489	-0.147287	0.061386	-0.017109
5.396668	0.000169	0.015689	0.619645	-0.330595	0.091847
2.678274	-0.000134	0.001047	0.613329	-0.579263	0.168375
1.187151	0.000069	-0.000117	0.088519	0.037342	-0.014436
0.596496	-0.000035	-0.000016	-0.004892	0.785367	-0.299678
0.271956	0.000011	-0.000034	0.002104	0.448424	-0.338238
0.055571	-0.000002	0.000003	-0.000243	0.011097	0.685965
0.022761	0.000001	-0.000002	0.000102	-0.003051	0.507698

p space			d space		
Exponent	2p	3p	4p	Exponent	3d
	-72.995973	-10.699918	-1.098122		-5.694336
35177.73	0.000051	-0.000021	0.000007	1225.269	0.000216
8327.432	0.000458	-0.000191	0.000061	369.9275	0.002069
2704.659	0.002641	-0.001104	0.000355	144.0983	0.011728
1034.889	0.011620	-0.004903	0.001578	63.70792	0.044768
439.2300	0.040985	-0.017571	0.005664	30.18951	0.124000
200.4365	0.115334	-0.051212	0.016605	14.95428	0.244771
96.29595	0.245586	-0.114300	0.037297	7.507677	0.337500
47.89735	0.360329	-0.179204	0.059252	3.762184	0.316465
24.38811	0.297283	-0.124339	0.039126	1.838006	0.162932
12.37563	0.101337	0.165377	-0.071128	0.815204	0.029469
6.199391	0.008814	0.473805	-0.203643		
3.098543	0.001284	0.410074	-0.209505		
1.492369	-0.000226	0.101519	0.112626		
0.712889	0.000144	0.002208	0.504564		
0.327674	-0.000064	0.001187	0.459367		
0.136821	0.000017	-0.000292	0.097978		

Table V. Sr 1S (26s16p10d) basis set. Energy(E_H) = -3131.545491

Exponent	s space				
	1s	2s	3s	4s	5s
	-583.687840	-80.390757	-13.474990	-1.896786	-0.178440
41610700.	0.000001	0.000000	0.000000	0.000000	0.000000
6386258.	0.000010	-0.000003	0.000001	0.000000	0.000000
1489632.	0.000050	-0.000016	0.000006	-0.000002	0.000001
432070.1	0.000205	-0.000065	0.000026	-0.000009	0.000002
144224.7	0.000725	-0.000230	0.000094	-0.000033	0.000009
53237.50	0.002300	-0.000730	0.000298	-0.000106	0.000027
21219.57	0.006676	-0.002128	0.000871	-0.000310	0.000080
8990.911	0.017889	-0.005760	0.002358	-0.000838	0.000216
4005.490	0.044118	-0.014541	0.005975	-0.002129	0.000550
1860.979	0.098304	-0.033890	0.014002	-0.004982	0.001284
895.8746	0.189476	-0.071610	0.029967	-0.010716	0.002768
444.5400	0.290668	-0.129991	0.055646	-0.019900	0.005129
226.1828	0.303294	-0.182401	0.081662	-0.029586	0.007665
116.7563	0.166202	-0.125391	0.059944	-0.021685	0.005570
58.25275	0.028810	0.176433	-0.098749	0.036432	-0.009359
30.93967	-0.000634	0.519069	-0.389234	0.155127	-0.040784
16.43147	0.000843	0.402314	-0.417610	0.171144	-0.044587
8.449350	-0.000456	0.088765	0.126451	-0.055872	0.013868
4.415150	0.000198	0.002481	0.689728	-0.421858	0.119291
2.294727	-0.000126	0.001743	0.448486	-0.485612	0.142984
1.047680	0.000065	-0.000564	0.050151	0.207920	-0.072983
0.533861	-0.000034	0.000206	-0.002648	0.750714	-0.293810
0.257330	0.000013	-0.000108	0.001594	0.367514	-0.317424
0.069611	-0.000005	0.000037	-0.000349	0.013967	0.374031
0.035727	0.000004	-0.000028	0.000259	-0.005639	0.615524
0.017363	-0.000001	0.000008	-0.000076	0.001291	0.219852
	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	-72.995990	-10.699935	-1.098136		-5.694353
35165.84	0.000051	-0.000021	0.000007	1225.266	0.000216
8324.613	0.000458	-0.000191	0.000061	369.9269	0.002069
2703.740	0.002643	-0.001105	0.000355	144.0982	0.011728
1034.536	0.011626	-0.004906	0.001579	63.70773	0.044769
439.0785	0.041007	-0.017581	0.005667	30.18912	0.124004
200.3660	0.115388	-0.051237	0.016613	14.95402	0.244772
96.26128	0.245667	-0.114341	0.037310	7.507688	0.337487
47.88019	0.360358	-0.179225	0.059259	3.762270	0.316464
24.37952	0.297193	-0.124244	0.039089	1.838043	0.162940
12.37107	0.101250	0.165559	-0.071195	0.815208	0.029470
6.197471	0.008797	0.473830	-0.203672		
3.097823	0.001285	0.409937	-0.209420		
1.492053	-0.000227	0.101458	0.112682		
0.712936	0.000144	0.002200	0.504380		
0.327775	-0.000064	0.001189	0.459356		
0.136906	0.000017	-0.000292	0.098133		

Table VI. Y^2D ($24s16p13d$) basis set. Energy(E_H) = -3331.683920

Exponent	s space				
	1s	2s	3s	4s	5s
	-616.749240	-85.810834	-14.758803	-2.168780	-0.196077
43596590.	0.000001	0.000000	0.000000	0.000000	0.000000
6533114.	0.000010	-0.000003	0.000001	-0.000001	0.000000
1487419.	0.000054	-0.000017	0.000007	-0.000003	0.000001
421417.1	0.000230	-0.000073	0.000030	-0.000011	0.000003
137508.7	0.000839	-0.000266	0.000110	-0.000040	0.000011
49649.91	0.002738	-0.000871	0.000359	-0.000132	0.000035
19367.86	0.008157	-0.002610	0.001077	-0.000396	0.000105
8035.047	0.022363	-0.007240	0.002991	-0.001101	0.000293
3506.130	0.056015	-0.018661	0.007741	-0.002851	0.000755
1595.790	0.124881	-0.044006	0.018381	-0.006781	0.001805
752.5103	0.233546	-0.092453	0.039257	-0.014513	0.003842
365.6377	0.326147	-0.160204	0.070094	-0.026074	0.006961
181.8739	0.273030	-0.190119	0.088077	-0.033026	0.008713
91.54202	0.093939	-0.028555	0.014050	-0.005501	0.001639
45.84816	0.006017	0.388036	-0.246427	0.098194	-0.026723
23.64228	0.000880	0.546181	-0.502770	0.212154	-0.056589
12.17258	-0.000406	0.215238	-0.164685	0.072459	-0.021271
5.852706	0.000161	0.017515	0.610754	-0.340860	0.099069
2.934943	-0.000133	0.000853	0.624470	-0.612560	0.182966
1.326419	0.000070	-0.000048	0.095139	0.040731	-0.012564
0.672837	-0.000034	-0.000060	-0.004548	0.802445	-0.332539
0.310211	0.000011	-0.000025	0.002147	0.443743	-0.328922
0.066292	-0.000002	0.000001	-0.000233	0.011851	0.674489
0.026451	0.000001	-0.000001	0.000094	-0.002987	0.525367

p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-78.164355	-11.854080	-1.301095		-6.599366	-0.249805
38140.68	0.000049	-0.000021	0.000007	1308.809	0.000217	-0.000047
9028.756	0.000438	-0.000184	0.000062	395.2284	0.002082	-0.000452
2932.495	0.002526	-0.001068	0.000359	153.9925	0.011828	-0.002565
1122.162	0.011136	-0.004749	0.001599	68.11930	0.045313	-0.009916
476.3737	0.039417	-0.017076	0.005761	32.31205	0.125809	-0.027719
217.4601	0.111608	-0.050047	0.016986	16.02608	0.248324	-0.054932
104.5465	0.240042	-0.112845	0.038549	8.061876	0.341277	-0.071862
52.05681	0.357724	-0.179668	0.062227	4.057269	0.313941	-0.058737
26.55320	0.302931	-0.131640	0.043654	1.997135	0.153758	0.044452
13.52904	0.107932	0.152894	-0.070022	0.902325	0.025685	0.245534
6.805144	0.010155	0.470863	-0.213950	0.384519	0.000051	0.410257
3.423491	0.001261	0.418444	-0.225282	0.155990	0.000349	0.390140
1.665507	-0.000213	0.106542	0.117272	0.058653	-0.000073	0.167756
0.804071	0.000132	0.002716	0.521241			
0.372820	-0.000062	0.001180	0.450142			
0.155127	0.000015	-0.000261	0.090120			

Table VII. Y^2D ($26s16p13d$) basis set. Energy(E_H) = -3331.683964

Exponent	s space					
	1s	2s	3s	4s	5s	
	-616.749270	-85.810860	-14.758829	-2.168803	-0.196103	
66514400.	0.000001	0.000000	0.000000	0.000000	0.000000	
10007620.	0.000006	-0.000002	0.000001	0.000000	0.000000	
2286245.	0.000032	-0.000010	0.000004	-0.000002	0.000000	
649996.8	0.000134	-0.000042	0.000017	-0.000006	0.000002	
212821.9	0.000485	-0.000154	0.000063	-0.000023	0.000006	
77096.71	0.001579	-0.000501	0.000207	-0.000076	0.000020	
30170.05	0.004705	-0.001500	0.000619	-0.000228	0.000060	
12554.56	0.012981	-0.004172	0.001722	-0.000633	0.000168	
5494.456	0.033144	-0.010845	0.004487	-0.001654	0.000439	
2508.387	0.077228	-0.026207	0.010894	-0.004010	0.001064	
1186.818	0.158488	-0.057935	0.024329	-0.008992	0.002390	
578.7628	0.266899	-0.112434	0.048131	-0.017798	0.004722	
289.3496	0.321661	-0.175686	0.078144	-0.029201	0.007781	
146.8534	0.217932	-0.164833	0.077988	-0.029235	0.007749	
73.29136	0.052339	0.072498	-0.039198	0.014633	-0.003817	
38.57178	0.000032	0.468067	-0.324322	0.131924	-0.035675	
20.32457	0.001395	0.481572	-0.478259	0.202875	-0.054566	
10.56379	-0.000712	0.145285	-0.030664	0.014540	-0.004849	
5.346448	0.000330	0.008239	0.659410	-0.390797	0.112888	
2.741508	-0.000212	0.001681	0.549243	-0.571819	0.174530	
1.254612	0.000115	-0.000486	0.075492	0.116711	-0.045601	
0.646469	-0.000063	0.000163	-0.004171	0.780026	-0.314705	
0.307816	0.000024	-0.000100	0.002211	0.415830	-0.335613	
0.084311	-0.000009	0.000032	-0.000494	0.018215	0.346121	
0.042746	0.000007	-0.000024	0.000356	-0.006859	0.626303	
0.020227	-0.000002	0.000007	-0.000102	0.001547	0.239746	
	p space			d space		
Exponent	2p	3p	4p	Exponent	3d	4d
	-78.164379	-11.854103	-1.301116		-6.599390	-0.249830
38102.21	0.000049	-0.000021	0.000007	1308.260	0.000217	-0.000047
9019.935	0.000438	-0.000185	0.000062	395.0789	0.002084	-0.000452
2929.754	0.002530	-0.001069	0.000359	153.9385	0.011836	-0.002567
1121.169	0.011152	-0.004756	0.001602	68.09629	0.045338	-0.009921
475.9737	0.039465	-0.017098	0.005768	32.30125	0.125863	-0.027730
217.2858	0.111720	-0.050100	0.017004	16.02067	0.248388	-0.054946
104.4656	0.240203	-0.112927	0.038577	8.059176	0.341295	-0.071861
52.01817	0.357782	-0.179710	0.062243	4.055961	0.313883	-0.058717
26.53428	0.302748	-0.131456	0.043580	1.996474	0.153677	0.044531
13.51933	0.107751	0.153261	-0.070168	0.901961	0.025655	0.245633
6.800776	0.010120	0.470975	-0.214035	0.384380	0.000049	0.410213
3.421625	0.001262	0.418165	-0.225118	0.155963	0.000349	0.390040
1.664617	-0.000214	0.106379	0.117565	0.058651	-0.000073	0.167738
0.803790	0.000133	0.002701	0.521219			
0.372759	-0.000062	0.001181	0.449930			
0.155147	0.000015	-0.000261	0.090130			

Table VIII. Zr 3F ($24s16p13d$) basis set. Energy(E_H) = -3538.994784

s space						
Exponent	1s	2s	3s	4s	5s	
	-650.704880	-91.377596	-16.054933	-2.419109	-0.207254	
31744170.	0.000002	-0.000001	0.000000	0.000000	0.000000	
4753203.	0.000016	-0.000005	0.000002	-0.000001	0.000000	
1081780.	0.000086	-0.000027	0.000011	-0.000004	0.000001	
306450.0	0.000365	-0.000116	0.000048	-0.000018	0.000005	
99993.28	0.001330	-0.000423	0.000176	-0.000066	0.000018	
36106.30	0.004328	-0.001383	0.000575	-0.000217	0.000058	
14085.96	0.012828	-0.004125	0.001714	-0.000647	0.000172	
5844.448	0.034706	-0.011388	0.004752	-0.001799	0.000478	
2550.568	0.084549	-0.028796	0.012056	-0.004555	0.001207	
1161.018	0.177688	-0.065896	0.027967	-0.010624	0.002823	
547.7010	0.295724	-0.128494	0.055604	-0.021113	0.005595	
266.2190	0.328190	-0.193140	0.087757	-0.033795	0.009009	
131.7147	0.182018	-0.135728	0.065612	-0.025242	0.006668	
61.27477	0.027764	0.225393	-0.130769	0.051775	-0.013717	
31.41355	-0.001847	0.570219	-0.465990	0.200415	-0.054397	
16.03042	0.001101	0.350071	-0.359506	0.158746	-0.042650	
7.388141	-0.000628	0.047042	0.427362	-0.222461	0.060663	
3.767080	0.000347	-0.002711	0.729244	-0.646767	0.198855	
1.866355	-0.000194	0.001799	0.190686	-0.184166	0.048786	
0.864156	0.000094	-0.000810	0.004830	0.774282	-0.289934	
0.391898	-0.000036	0.000238	0.001516	0.569243	-0.392369	
0.108075	0.000018	-0.000130	-0.000186	0.036092	0.135833	
0.059320	-0.000013	0.000093	0.000145	-0.013508	0.674455	
0.025360	0.000003	-0.000022	-0.000034	0.002295	0.381442	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-83.478445	-13.019674	-1.487517		-7.515746	-0.336709
41243.02	0.000047	-0.000020	0.000007	1411.630	0.000212	-0.000052
9762.892	0.000419	-0.000178	0.000062	426.3812	0.002041	-0.000502
3170.935	0.002421	-0.001034	0.000360	166.1773	0.011645	-0.002860
1213.477	0.010694	-0.004606	0.001605	73.56633	0.044886	-0.011132
515.2322	0.037976	-0.016614	0.005800	34.94158	0.125343	-0.031311
235.2683	0.108152	-0.048945	0.017194	17.36324	0.248739	-0.062457
113.1791	0.234790	-0.111411	0.039397	8.762151	0.342961	-0.081805
56.41261	0.355008	-0.179942	0.064541	4.434854	0.313154	-0.065336
28.82333	0.308044	-0.138344	0.047770	2.204806	0.149746	0.056223
14.74010	0.114378	0.140900	-0.068001	1.015825	0.024518	0.273631
7.442160	0.011572	0.467543	-0.221778	0.448575	0.000193	0.420835
3.766226	0.001232	0.426408	-0.238952	0.189892	0.000340	0.357754
1.848848	-0.000195	0.111551	0.119793	0.074305	-0.000055	0.132133
0.899601	0.000116	0.003334	0.530974			
0.419026	-0.000060	0.001196	0.444916			
0.174769	0.000013	-0.000233	0.087211			

Table IX. Zr 3F (24s16p13d) basis set. Energy(E_H) = -3538.994805

Exponent	s space					
	1s	2s	3s	4s	5s	
	-650.704870	-91.377581	-16.054918	-2.419099	-0.207225	
47457370.	0.000001	0.000000	0.000000	0.000000	0.000000	
7096971.	0.000010	-0.000003	0.000001	-0.000001	0.000000	
1613921.	0.000052	-0.000017	0.000007	-0.000003	0.000001	
456939.0	0.000222	-0.000070	0.000029	-0.000011	0.000003	
149035.3	0.000809	-0.000257	0.000107	-0.000040	0.000011	
53799.19	0.002640	-0.000841	0.000349	-0.000132	0.000035	
20984.05	0.007869	-0.002523	0.001049	-0.000396	0.000105	
8705.072	0.021593	-0.007002	0.002914	-0.001102	0.000293	
3798.439	0.054184	-0.018070	0.007554	-0.002856	0.000756	
1728.898	0.121259	-0.042700	0.017967	-0.006807	0.001811	
815.4182	0.228428	-0.090123	0.038550	-0.014632	0.003868	
396.3950	0.323583	-0.157464	0.069332	-0.026486	0.007071	
197.4625	0.278316	-0.191449	0.089233	-0.034349	0.009045	
99.82205	0.101407	-0.041532	0.020656	-0.008256	0.002401	
49.70794	0.007674	0.371389	-0.235650	0.096494	-0.026322	
25.65954	0.000645	0.551726	-0.505927	0.219364	-0.058405	
13.24254	-0.000283	0.229980	-0.190678	0.087445	-0.025668	
6.350395	0.000098	0.020151	0.601103	-0.347463	0.101785	
3.204205	-0.000101	0.000528	0.638669	-0.643625	0.192377	
1.461988	0.000053	0.000076	0.100644	0.050058	-0.015055	
0.744718	-0.000025	-0.000128	-0.004394	0.816324	-0.347126	
0.344328	0.000009	-0.000007	0.002203	0.435285	-0.313214	
0.074055	-0.000002	-0.000003	-0.000229	0.011643	0.664742	
0.028972	0.000001	0.000001	0.000091	-0.002851	0.533146	
	p space			d space		
Exponent	2p	3p	4p	Exponent	3d	4d
	-83.478428	-13.019657	-1.487502		-7.515729	-0.336691
41213.72	0.000047	-0.000020	0.000007	1410.391	0.000212	-0.000052
9755.642	0.000420	-0.000179	0.000062	426.0443	0.002044	-0.000503
3168.514	0.002425	-0.001035	0.000360	166.0570	0.011660	-0.002864
1212.532	0.010708	-0.004612	0.001607	73.51640	0.044934	-0.011144
514.8240	0.038023	-0.016634	0.005807	34.91917	0.125443	-0.031336
235.0797	0.108268	-0.048999	0.017213	17.35216	0.248867	-0.062490
113.0855	0.234983	-0.111510	0.039432	8.756303	0.343020	-0.081813
56.36324	0.355138	-0.180022	0.064572	4.431865	0.313034	-0.065288
28.79582	0.307868	-0.138141	0.047683	2.203302	0.149572	0.056410
14.72383	0.114118	0.141523	-0.068261	1.015056	0.024460	0.273825
7.432949	0.011506	0.467991	-0.222059	0.448233	0.000191	0.420912
3.761160	0.001232	0.425934	-0.238661	0.189728	0.000340	0.357572
1.845680	-0.000197	0.111074	0.120909	0.074245	-0.000054	0.131892
0.898215	0.000117	0.003269	0.531146			
0.418532	-0.000060	0.001200	0.444160			
0.174574	0.000013	-0.000234	0.086919			

Table X. Zr 3F (26s16p13d) basis set. Energy(E_H) = -3538.994855

Exponent	s space					
	1s	2s	3s	4s	5s	
	-650.704910	-91.377615	-16.054952	-2.419128	-0.207258	
69038840.	0.000001	0.000000	0.000000	0.000000	0.000000	
10374700.	0.000006	-0.000002	0.000001	0.000000	0.000000	
2376150.	0.000032	-0.000010	0.000004	-0.000002	0.000000	
677705.0	0.000135	-0.000043	0.000018	-0.000007	0.000002	
222475.3	0.000488	-0.000155	0.000064	-0.000024	0.000006	
80750.63	0.001585	-0.000505	0.000210	-0.000079	0.000021	
31651.79	0.004714	-0.001506	0.000626	-0.000237	0.000063	
13194.71	0.012970	-0.004178	0.001738	-0.000656	0.000174	
5786.927	0.033013	-0.010826	0.004514	-0.001708	0.000453	
2648.232	0.076704	-0.026087	0.010930	-0.004131	0.001095	
1256.109	0.157131	-0.057532	0.024348	-0.009241	0.002455	
614.0702	0.264743	-0.111596	0.048152	-0.018284	0.004846	
307.7358	0.320741	-0.174774	0.078325	-0.030063	0.008007	
156.6009	0.220267	-0.166533	0.079416	-0.030580	0.008097	
78.63402	0.054669	0.063617	-0.034728	0.013253	-0.003437	
41.45708	0.000395	0.458942	-0.318704	0.133318	-0.036066	
21.91215	0.001363	0.487476	-0.484681	0.211575	-0.056902	
11.45831	-0.000695	0.154529	-0.052632	0.026163	-0.008155	
5.808423	0.000321	0.009675	0.653693	-0.401095	0.116377	
3.000664	-0.000213	0.001563	0.562518	-0.600409	0.183958	
1.399124	0.000115	-0.000444	0.081341	0.120969	-0.048112	
0.720505	-0.000061	0.000126	-0.003526	0.792857	-0.325381	
0.343503	0.000023	-0.000089	0.002173	0.412881	-0.325359	
0.096572	-0.000009	0.000027	-0.000451	0.018186	0.325353	
0.047947	0.000006	-0.000019	0.000313	-0.006251	0.633658	
0.022216	-0.000002	0.000006	-0.000089	0.001389	0.252392	
	p space			d space		
Exponent	2p	3p	4p	Exponent	3d	4d
	-83.478460	-13.019689	-1.487531		-7.515761	-0.336722
41044.17	0.000047	-0.000020	0.000007	1407.513	0.000213	-0.000052
9718.603	0.000422	-0.000180	0.000063	425.2386	0.002052	-0.000505
3157.576	0.002438	-0.001041	0.000362	165.7699	0.011698	-0.002873
1208.795	0.010758	-0.004634	0.001615	73.39894	0.045045	-0.011172
513.4156	0.038167	-0.016699	0.005830	34.86735	0.125666	-0.031393
234.5106	0.108570	-0.049143	0.017264	17.32811	0.249094	-0.062543
112.8429	0.235368	-0.111711	0.039503	8.745124	0.343043	-0.081810
56.25626	0.355230	-0.180100	0.064605	4.426912	0.312761	-0.065178
28.74669	0.307399	-0.137706	0.047504	2.201197	0.149286	0.056628
14.69990	0.113683	0.142373	-0.068610	1.014305	0.024390	0.273932
7.421770	0.011421	0.468347	-0.222312	0.448023	0.000192	0.420755
3.755980	0.001231	0.425307	-0.238277	0.189701	0.000338	0.357444
1.842938	-0.000199	0.110624	0.121840	0.074246	-0.000054	0.131891
0.897088	0.000118	0.003222	0.531304			
0.418115	-0.000060	0.001202	0.443491			
0.174450	0.000014	-0.000235	0.086712			

Table XI. Zr 3F (26s16p13d) basis set. Energy(E_H) = -3538.994855

Exponent	s space					
	1s	2s	3s	4s	5s	
	-650.704910	-91.377616	-16.054953	-2.419129	-0.207258	
66667890.	0.000001	0.000000	0.000000	0.000000	0.000000	
10059580.	0.000006	-0.000002	0.000001	0.000000	0.000000	
2308569.	0.000033	-0.000011	0.000004	-0.000002	0.000000	
659417.3	0.000139	-0.000044	0.000018	-0.000007	0.000002	
216834.4	0.000503	-0.000160	0.000066	-0.000025	0.000007	
78857.43	0.001629	-0.000519	0.000215	-0.000081	0.000022	
30973.99	0.004831	-0.001544	0.000642	-0.000243	0.000064	
12936.06	0.013261	-0.004272	0.001777	-0.000671	0.000178	
5681.443	0.033686	-0.011054	0.004610	-0.001744	0.000463	
2602.538	0.078093	-0.026589	0.011141	-0.004211	0.001116	
1235.339	0.159424	-0.058513	0.024772	-0.009403	0.002498	
604.3115	0.267035	-0.113040	0.048802	-0.018532	0.004911	
303.0463	0.320261	-0.175845	0.078900	-0.030294	0.008069	
154.2799	0.216422	-0.164188	0.078418	-0.030194	0.007992	
77.28962	0.052169	0.072488	-0.039674	0.015198	-0.003950	
40.83573	0.000086	0.465163	-0.325649	0.136462	-0.036936	
21.60729	0.001385	0.481218	-0.481441	0.210252	-0.056518	
11.29707	-0.000714	0.148489	-0.039416	0.020213	-0.006604	
5.754975	0.000334	0.008872	0.657945	-0.406473	0.118181	
2.978631	-0.000218	0.001626	0.554962	-0.595630	0.182382	
1.387523	0.000117	-0.000478	0.079133	0.131152	-0.051346	
0.715797	-0.000063	0.000143	-0.003597	0.791213	-0.326118	
0.341967	0.000024	-0.000095	0.002171	0.407803	-0.322639	
0.096130	-0.000009	0.000029	-0.000451	0.017791	0.331845	
0.047571	0.000006	-0.000020	0.000313	-0.006119	0.632339	
0.022090	-0.000002	0.000006	-0.000090	0.001372	0.247599	
	p space			d space		
Exponent	2p	3p	4p	Exponent	3d	4d
	-83.478460	-13.019689	-1.487532		-7.515761	-0.336722
41110.33	0.000047	-0.000020	0.000007	1408.702	0.000213	-0.000052
9732.583	0.000421	-0.000179	0.000062	425.5463	0.002049	-0.000504
3161.307	0.002434	-0.001039	0.000361	165.8761	0.011684	-0.002870
1209.800	0.010748	-0.004629	0.001613	73.44281	0.045002	-0.011161
513.6666	0.038154	-0.016693	0.005827	34.88745	0.125574	-0.031370
234.5528	0.108587	-0.049150	0.017267	17.33794	0.248989	-0.062518
112.8317	0.235477	-0.111763	0.039521	8.749997	0.343015	-0.081806
56.23698	0.355384	-0.180186	0.064637	4.429198	0.312877	-0.065227
28.73092	0.307361	-0.137613	0.047460	2.202197	0.149420	0.056525
14.68876	0.113520	0.142806	-0.068787	1.014658	0.024423	0.273882
7.415312	0.011373	0.468669	-0.222522	0.448128	0.000191	0.420804
3.752355	0.001232	0.424983	-0.238056	0.189725	0.000339	0.357510
1.840564	-0.000201	0.110278	0.122643	0.074250	-0.000054	0.131911
0.896035	0.000119	0.003172	0.531522			
0.417676	-0.000061	0.001205	0.442905			
0.174265	0.000014	-0.000236	0.086441			

Table XII. Nb 4F ($24s16p13d$) basis set. Energy(E_H) = -3753.551742

Exponent	s space					
	1s	2s	3s	4s	5s	
	-685.571800	-97.109019	-17.381555	-2.665247	-0.216563	
33360650.	0.000002	-0.000001	0.000000	0.000000	0.000000	
4995325.	0.000016	-0.000005	0.000002	-0.000001	0.000000	
1136882.	0.000086	-0.000028	0.000012	-0.000004	0.000001	
322059.3	0.000365	-0.000116	0.000049	-0.000019	0.000005	
105087.2	0.001330	-0.000424	0.000177	-0.000068	0.000018	
37946.25	0.004328	-0.001386	0.000580	-0.000224	0.000059	
14804.08	0.012826	-0.004134	0.001731	-0.000668	0.000176	
6142.522	0.034701	-0.011411	0.004797	-0.001856	0.000488	
2680.692	0.084544	-0.028859	0.012172	-0.004702	0.001236	
1220.273	0.177700	-0.066058	0.028248	-0.010963	0.002887	
575.6739	0.295775	-0.128854	0.056189	-0.021823	0.005739	
279.8374	0.328219	-0.193697	0.088725	-0.034903	0.009214	
138.4868	0.181939	-0.135872	0.066247	-0.026144	0.006875	
64.46560	0.027700	0.227172	-0.133320	0.054256	-0.014328	
33.06166	-0.001848	0.571242	-0.472587	0.207952	-0.055864	
16.87583	0.001089	0.348643	-0.359972	0.164354	-0.044163	
7.772997	-0.000624	0.046226	0.445064	-0.242669	0.066680	
3.969563	0.000344	-0.002796	0.731978	-0.681580	0.208008	
1.943311	-0.000195	0.001768	0.176859	-0.146338	0.036786	
0.929096	0.000097	-0.000839	0.002447	0.804481	-0.306958	
0.421681	-0.000034	0.000229	0.001972	0.542319	-0.372558	
0.110417	0.000016	-0.000115	-0.000332	0.030708	0.220234	
0.058828	-0.000012	0.000085	0.000253	-0.012336	0.638660	
0.025933	0.000003	-0.000022	-0.000065	0.002398	0.335239	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-88.956110	-14.214850	-1.672194		-8.461241	-0.405818
44376.77	0.000045	-0.000019	0.000007	1508.399	0.000211	-0.000056
10503.94	0.000404	-0.000174	0.000062	455.7202	0.002030	-0.000540
3411.485	0.002336	-0.001007	0.000360	177.6602	0.011617	-0.003093
1305.556	0.010332	-0.004491	0.001610	78.69627	0.044969	-0.012083
554.4010	0.036795	-0.016246	0.005832	37.41669	0.126014	-0.034163
253.2146	0.105302	-0.048073	0.017368	18.61912	0.250613	-0.068230
121.8755	0.230413	-0.110313	0.040122	9.417129	0.345401	-0.089396
60.79934	0.352617	-0.180307	0.066550	4.787577	0.311239	-0.068487
31.10805	0.312134	-0.143904	0.051324	2.399213	0.143914	0.068110
15.95626	0.119853	0.131243	-0.066259	1.125821	0.022815	0.293693
8.081312	0.012840	0.465269	-0.228931	0.507577	0.000376	0.423394
4.110814	0.001198	0.432563	-0.250413	0.219253	0.000285	0.334710
2.032359	-0.000180	0.115153	0.124143	0.087274	-0.000030	0.113603
0.994893	0.000100	0.003836	0.538412			
0.465058	-0.000058	0.001227	0.439791			
0.194600	0.000012	-0.000208	0.084882			

Table XIII. Nb 4F ($24s16p13d$) basis set. Energy(E_H) = -3753.551759

s space						
Exponent	1s	2s	3s	4s	5s	
	-685.571790	-97.108995	-17.381531	-2.665226	-0.216525	
50854550.	0.000001	0.000000	0.000000	0.000000	0.000000	
7610525.	0.000010	-0.000003	0.000001	-0.000001	0.000000	
1731519.	0.000051	-0.000016	0.000007	-0.000003	0.000001	
490407.6	0.000216	-0.000069	0.000029	-0.000011	0.000003	
159994.0	0.000787	-0.000251	0.000105	-0.000041	0.000011	
57765.49	0.002570	-0.000821	0.000343	-0.000133	0.000035	
22533.76	0.007662	-0.002462	0.001031	-0.000398	0.000104	
9348.794	0.021034	-0.006832	0.002864	-0.001107	0.000292	
4079.686	0.052847	-0.017646	0.007431	-0.002871	0.000753	
1857.147	0.118582	-0.041759	0.017696	-0.006853	0.001808	
876.0966	0.224575	-0.088430	0.038094	-0.014775	0.003871	
426.0694	0.321491	-0.155475	0.068894	-0.026906	0.007125	
212.4535	0.282173	-0.192366	0.090220	-0.035486	0.009258	
107.6542	0.107138	-0.050782	0.025451	-0.010392	0.002966	
53.42339	0.008942	0.359025	-0.228293	0.095687	-0.025942	
27.60731	0.000487	0.555188	-0.508825	0.225653	-0.059539	
14.27257	-0.000203	0.241003	-0.209971	0.099672	-0.029025	
6.838947	0.000058	0.022189	0.595425	-0.355660	0.104023	
3.471221	-0.000079	0.000266	0.648501	-0.669782	0.198854	
1.596158	0.000042	0.000165	0.104276	0.065442	-0.020335	
0.813976	-0.000019	-0.000177	-0.004129	0.826348	-0.354369	
0.376999	0.000007	0.000005	0.002223	0.425067	-0.297539	
0.080885	-0.000001	-0.000005	-0.000222	0.011155	0.656696	
0.031135	0.000000	0.000002	0.000088	-0.002695	0.537688	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-88.956084	-14.214823	-1.672170		-8.461214	-0.405791
44339.12	0.000045	-0.000019	0.000007	1507.548	0.000211	-0.000056
10495.59	0.000404	-0.000174	0.000062	455.4542	0.002033	-0.000541
3408.913	0.002339	-0.001008	0.000360	177.5559	0.011630	-0.003097
1304.614	0.010344	-0.004496	0.001611	78.64993	0.045013	-0.012095
554.0152	0.036833	-0.016263	0.005838	37.39473	0.126111	-0.034190
253.0446	0.105392	-0.048116	0.017384	18.60789	0.250740	-0.068264
121.7948	0.230559	-0.110389	0.040150	9.411186	0.345453	-0.089405
60.75826	0.352711	-0.180366	0.066573	4.784584	0.311116	-0.068428
31.08584	0.311999	-0.143756	0.051260	2.397748	0.143752	0.068284
15.94351	0.119656	0.131694	-0.066453	1.125146	0.022767	0.293831
8.074216	0.012788	0.465592	-0.229138	0.507276	0.000376	0.423444
4.106997	0.001197	0.432219	-0.250196	0.219102	0.000284	0.334547
2.030057	-0.000182	0.114819	0.124914	0.087220	-0.000030	0.113429
0.993922	0.000101	0.003793	0.538451			
0.464737	-0.000058	0.001230	0.439323			
0.194470	0.000012	-0.000209	0.084713			

Table XIV. Nb $4F$ ($26s16p13d$) basis set. Energy(E_H) = -3753.551816

s space						
Exponent	1s	2s	3s	4s	5s	
	-685.571840	-97.109036	-17.381571	-2.665262	-0.216565	
79385660.	0.000001	0.000000	0.000000	0.000000	0.000000	
11903180.	0.000006	-0.000002	0.000001	0.000000	0.000000	
2715073.	0.000029	-0.000009	0.000004	-0.000002	0.000000	
770918.2	0.000122	-0.000039	0.000016	-0.000006	0.000002	
252129.5	0.000445	-0.000142	0.000059	-0.000023	0.000006	
91231.21	0.001452	-0.000463	0.000194	-0.000075	0.000020	
35656.16	0.004339	-0.001389	0.000581	-0.000225	0.000059	
14818.14	0.012006	-0.003873	0.001623	-0.000626	0.000165	
6476.749	0.030783	-0.010096	0.004239	-0.001639	0.000431	
2953.130	0.072214	-0.024524	0.010347	-0.003997	0.001050	
1395.549	0.149952	-0.054613	0.023260	-0.009021	0.002376	
679.7782	0.257724	-0.107463	0.046641	-0.018099	0.004756	
339.5680	0.322106	-0.171950	0.077387	-0.030346	0.008013	
172.4837	0.232141	-0.173447	0.083013	-0.032677	0.008581	
87.09748	0.062838	0.038378	-0.021122	0.008063	-0.002032	
45.70637	0.001381	0.438758	-0.301045	0.128483	-0.034480	
24.13437	0.001332	0.503987	-0.495665	0.221327	-0.059068	
12.66053	-0.000672	0.174151	-0.094743	0.047468	-0.013926	
6.376382	0.000309	0.012490	0.640702	-0.400949	0.115596	
3.304552	-0.000212	0.001338	0.586703	-0.633112	0.192930	
1.560714	0.000115	-0.000345	0.090044	0.112699	-0.046143	
0.800631	-0.000059	0.000064	-0.002963	0.805740	-0.330215	
0.380069	0.000022	-0.000070	0.002163	0.415877	-0.316864	
0.105443	-0.000008	0.000019	-0.000416	0.018082	0.326181	
0.051548	0.000006	-0.000013	0.000289	-0.006215	0.629380	
0.023660	-0.000002	0.000004	-0.000083	0.001407	0.251967	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-88.956122	-14.214861	-1.672205		-8.461252	-0.405829
44271.30	0.000046	-0.000020	0.000007	1507.187	0.000211	-0.000056
10480.12	0.000405	-0.000174	0.000062	455.3497	0.002034	-0.000541
3404.070	0.002344	-0.001010	0.000361	177.5183	0.011635	-0.003098
1302.833	0.010367	-0.004506	0.001615	78.63500	0.045025	-0.012098
553.2925	0.036904	-0.016295	0.005849	37.38841	0.126136	-0.034197
252.7296	0.105558	-0.048195	0.017413	18.60511	0.250760	-0.068268
121.6492	0.230805	-0.110516	0.040196	9.410093	0.345440	-0.089400
60.68874	0.352820	-0.180442	0.066604	4.784258	0.311081	-0.068414
31.05167	0.311737	-0.143498	0.051150	2.397700	0.143736	0.068280
15.92598	0.119362	0.132273	-0.066700	1.125206	0.022768	0.293789
8.066034	0.012724	0.465846	-0.229322	0.507357	0.000376	0.423355
4.103255	0.001198	0.431789	-0.249925	0.219168	0.000284	0.334602
2.028146	-0.000183	0.114515	0.125537	0.087245	-0.000030	0.113509
0.993119	0.000101	0.003763	0.538549			
0.464437	-0.000059	0.001230	0.438872			
0.194393	0.000012	-0.000209	0.084591			

Table XV. Mo 5D (24s16p13d) basis set. Energy(E_H) = -3975.443022

Exponent	s space					
	1s	2s	3s	4s	5s	
	-721.352270	-103.007520	-18.741420	-2.910107	-0.224626	
35112180.	0.000002	-0.000001	0.000000	0.000000	0.000000	
5258106.	0.000016	-0.000005	0.000002	-0.000001	0.000000	
1196801.	0.000086	-0.000027	0.000012	-0.000005	0.000001	
339059.4	0.000364	-0.000116	0.000049	-0.000019	0.000005	
110640.9	0.001325	-0.000423	0.000178	-0.000070	0.000018	
39953.40	0.004311	-0.001383	0.000583	-0.000230	0.000060	
15587.64	0.012776	-0.004126	0.001739	-0.000684	0.000177	
6467.834	0.034571	-0.011391	0.004822	-0.001899	0.000493	
2822.765	0.084252	-0.028816	0.012238	-0.004817	0.001250	
1285.011	0.177204	-0.065993	0.028419	-0.011230	0.002918	
606.2569	0.295318	-0.128858	0.056592	-0.022402	0.005820	
294.7315	0.328476	-0.194040	0.089538	-0.035861	0.009338	
145.8847	0.182790	-0.136874	0.067260	-0.027120	0.007061	
67.96261	0.027993	0.226316	-0.134114	0.055849	-0.014613	
34.88161	-0.001875	0.571567	-0.477304	0.214105	-0.056723	
17.81393	0.001099	0.349625	-0.363562	0.170847	-0.045608	
8.210759	-0.000631	0.046252	0.455443	-0.258153	0.070818	
4.206072	0.000349	-0.002907	0.734863	-0.709907	0.214184	
2.043685	-0.000198	0.001756	0.169232	-0.114148	0.025863	
0.996150	0.000100	-0.000860	0.001004	0.824340	-0.316229	
0.452624	-0.000034	0.000224	0.002240	0.520742	-0.353871	
0.114939	0.000015	-0.000104	-0.000392	0.026798	0.270466	
0.059130	-0.000011	0.000077	0.000297	-0.010995	0.620669	
0.026463	0.000003	-0.000021	-0.000081	0.002354	0.302033	
	p space			d space		
Exponent	2p	3p	4p	Exponent	3d	4d
	-94.599758	-15.442374	-1.857297		-9.438458	-0.469958
47638.24	0.000044	-0.000019	0.000007	1606.556	0.000210	-0.000059
11275.44	0.000390	-0.000169	0.000062	485.3496	0.002026	-0.000572
3661.925	0.002256	-0.000981	0.000359	189.2169	0.011626	-0.003288
1401.406	0.009998	-0.004384	0.001608	83.84253	0.045182	-0.012885
595.1657	0.035700	-0.015899	0.005842	39.89246	0.126997	-0.036612
271.8887	0.102642	-0.047244	0.017474	19.87089	0.252930	-0.073131
130.9236	0.226273	-0.109237	0.040680	10.06666	0.348125	-0.095810
65.36412	0.350230	-0.180563	0.068262	5.135102	0.309083	-0.069914
33.48602	0.315867	-0.149052	0.054637	2.588562	0.137743	0.080304
17.22222	0.125133	0.122070	-0.064223	1.233712	0.020980	0.309586
8.746748	0.014126	0.462943	-0.235035	0.564722	0.000526	0.422434
4.470095	0.001161	0.438313	-0.260758	0.247233	0.000215	0.316224
2.223903	-0.000163	0.118644	0.127583	0.099485	-0.000011	0.101076
1.093599	0.000082	0.004372	0.543898			
0.512496	-0.000056	0.001262	0.436188			
0.215183	0.000010	-0.000184	0.083459			

Table XVI. Mo $5D$ ($24s16p13d$) basis set. Energy(E_H) = -3975.443036

Exponent	s space					
	1s	2s	3s	4s	5s	
	-721.352250	-103.007490	-18.741387	-2.910075	-0.224582	
54327360.	0.000001	0.000000	0.000000	0.000000	0.000000	
8130625.	0.000010	-0.000003	0.000001	-0.000001	0.000000	
1850196.	0.000050	-0.000016	0.000007	-0.000003	0.000001	
524081.9	0.000211	-0.000067	0.000028	-0.000011	0.000003	
170991.1	0.000770	-0.000246	0.000104	-0.000041	0.000011	
61738.34	0.002513	-0.000804	0.000339	-0.000133	0.000035	
24084.37	0.007492	-0.002412	0.001017	-0.000400	0.000104	
9992.615	0.020578	-0.006695	0.002826	-0.001112	0.000289	
4360.984	0.051750	-0.017302	0.007337	-0.002887	0.000747	
1985.448	0.116372	-0.040995	0.017489	-0.006899	0.001797	
936.8258	0.221345	-0.087045	0.037749	-0.014911	0.003856	
455.7805	0.319619	-0.153831	0.068587	-0.027291	0.007137	
227.4602	0.285262	-0.193041	0.091088	-0.036484	0.009393	
115.4687	0.112048	-0.058314	0.029421	-0.012239	0.003425	
57.14983	0.010085	0.348534	-0.222325	0.095071	-0.025493	
29.56754	0.000341	0.557616	-0.511407	0.231179	-0.060206	
15.31043	-0.000128	0.250427	-0.226409	0.110644	-0.031809	
7.334974	0.000020	0.024018	0.591088	-0.363711	0.105620	
3.744420	-0.000058	0.000015	0.656430	-0.692369	0.203271	
1.734868	0.000030	0.000246	0.107351	0.081084	-0.025990	
0.883574	-0.000013	-0.000221	-0.003739	0.833758	-0.356573	
0.409476	0.000005	0.000016	0.002216	0.415931	-0.283601	
0.087073	-0.000001	-0.000007	-0.000212	0.010624	0.649576	
0.033058	0.000000	0.000003	0.000083	-0.002560	0.540567	
	p space			d space		
Exponent	2p	3p	4p	Exponent	3d	4d
	-94.599723	-15.442339	-1.857264		-9.438423	-0.469922
47515.14	0.000044	-0.000019	0.000007	1601.820	0.000211	-0.000059
11247.10	0.000392	-0.000170	0.000062	484.0744	0.002037	-0.000575
3653.006	0.002266	-0.000985	0.000361	188.7689	0.011677	-0.003303
1398.102	0.010036	-0.004401	0.001614	83.65927	0.045337	-0.012930
593.8058	0.035823	-0.015955	0.005862	39.81101	0.127316	-0.036706
271.2865	0.102937	-0.047385	0.017527	19.83186	0.253300	-0.073233
130.6394	0.226738	-0.109480	0.040770	10.04706	0.348252	-0.095830
65.22330	0.350502	-0.180741	0.068336	5.125284	0.308696	-0.069692
33.41302	0.315427	-0.148591	0.054431	2.583623	0.137244	0.080864
17.18230	0.124528	0.123340	-0.064779	1.231460	0.020837	0.309992
8.726223	0.013970	0.463739	-0.235583	0.563738	0.000525	0.422386
4.459627	0.001161	0.437375	-0.260125	0.246814	0.000212	0.315717
2.217841	-0.000168	0.117797	0.129476	0.099347	-0.000010	0.100723
1.090975	0.000084	0.004267	0.544115			
0.511494	-0.000057	0.001266	0.434993			
0.214771	0.000010	-0.000186	0.082978			

Table XVII. Mo 5D ($26s16p13d$) basis set. Energy(E_H) = -3975.443098

Exponent	s space				
	1s	2s	3s	4s	5s
	-721.352300	-103.007540	-18.741435	-2.910119	-0.224628
80164450.	0.000001	0.000000	0.000000	0.000000	0.000000
12058280.	0.000006	-0.000002	0.000001	0.000000	0.000000
2761403.	0.000030	-0.000010	0.000004	-0.000002	0.000000
786769.1	0.000127	-0.000040	0.000017	-0.000007	0.000002
258067.9	0.000458	-0.000146	0.000062	-0.000024	0.000006
93651.51	0.001489	-0.000476	0.000201	-0.000079	0.000020
36711.92	0.004429	-0.001421	0.000599	-0.000236	0.000061
15302.43	0.012205	-0.003946	0.001665	-0.000654	0.000170
6707.514	0.031169	-0.010248	0.004333	-0.001707	0.000444
3066.441	0.072842	-0.024807	0.010541	-0.004147	0.001076
1452.640	0.150680	-0.055064	0.023621	-0.009333	0.002427
709.2059	0.257974	-0.108004	0.047227	-0.018667	0.004842
355.0448	0.321210	-0.172257	0.078127	-0.031224	0.008142
180.7364	0.230926	-0.173064	0.083522	-0.033491	0.008680
91.47046	0.062548	0.039032	-0.021734	0.008426	-0.002090
48.15073	0.001381	0.437621	-0.303372	0.132300	-0.035094
25.49632	0.001333	0.503283	-0.498918	0.227387	-0.059929
13.41891	-0.000678	0.175698	-0.098926	0.051752	-0.015075
6.797348	0.000316	0.012763	0.643338	-0.416916	0.119357
3.547379	-0.000217	0.001324	0.587923	-0.649743	0.195924
1.693238	0.000116	-0.000364	0.091303	0.134560	-0.054086
0.866610	-0.000058	0.000062	-0.002365	0.812330	-0.332205
0.411717	0.000022	-0.000070	0.002084	0.404411	-0.302551
0.113975	-0.000008	0.000018	-0.000374	0.016893	0.326250
0.054781	0.000005	-0.000013	0.000257	-0.005673	0.627100
0.024912	-0.000002	0.000004	-0.000075	0.001300	0.250883

p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-94.599768	-15.442384	-1.857306		-9.438468	-0.469966
47421.43	0.000044	-0.000019	0.000007	1599.612	0.000212	-0.000059
11226.94	0.000393	-0.000170	0.000062	483.4492	0.002042	-0.000577
3647.034	0.002272	-0.000988	0.000362	188.5423	0.011703	-0.003310
1396.013	0.010059	-0.004411	0.001618	83.56431	0.045419	-0.012953
592.9910	0.035894	-0.015987	0.005874	39.76778	0.127490	-0.036757
270.9414	0.103100	-0.047464	0.017557	19.81087	0.253499	-0.073286
130.4827	0.226978	-0.109606	0.040817	10.03665	0.348307	-0.095838
65.14934	0.350612	-0.180818	0.068368	5.120196	0.308483	-0.069569
33.37698	0.315173	-0.148345	0.054323	2.581142	0.136986	0.081131
17.16400	0.124234	0.123903	-0.065026	1.230433	0.020767	0.310140
8.717779	0.013903	0.463988	-0.235765	0.563367	0.000526	0.422243
4.455846	0.001162	0.436954	-0.259855	0.246704	0.000211	0.315553
2.216004	-0.000169	0.117512	0.130059	0.099311	-0.000010	0.100643
1.090176	0.000084	0.004241	0.544200			
0.511192	-0.000057	0.001265	0.434578			
0.214693	0.000010	-0.000186	0.082868			

Table XVIII. Tc 6S ($24s16p13d$) basis set. Energy(E_H) = -4204.788431

s space						
Exponent	1s	2s	3s	4s	5s	
	-758.042950	-109.069700	-20.131750	-3.152118	-0.231240	
37369900.	0.000002	-0.000001	0.000000	0.000000	0.000000	
5593742.	0.000016	-0.000005	0.000002	-0.000001	0.000000	
1272680.	0.000085	-0.000027	0.000011	-0.000005	0.000001	
360416.4	0.000358	-0.000114	0.000049	-0.000019	0.000005	
117566.3	0.001303	-0.000417	0.000177	-0.000071	0.000018	
42439.13	0.004243	-0.001364	0.000579	-0.000231	0.000059	
16551.81	0.012584	-0.004071	0.001727	-0.000690	0.000176	
6865.657	0.034082	-0.011247	0.004793	-0.001917	0.000489	
2995.442	0.083188	-0.028487	0.012177	-0.004869	0.001242	
1363.203	0.175433	-0.065360	0.028328	-0.011367	0.002902	
642.9433	0.293747	-0.128057	0.056598	-0.022764	0.005811	
312.4508	0.329488	-0.194017	0.090089	-0.036636	0.009373	
154.5859	0.185867	-0.139897	0.069201	-0.028396	0.007267	
72.06435	0.029070	0.220133	-0.131307	0.055688	-0.014324	
37.02959	-0.001955	0.570850	-0.478820	0.218278	-0.056845	
18.92075	0.001150	0.355344	-0.373192	0.179524	-0.047177	
8.731869	-0.000663	0.047827	0.454092	-0.264905	0.071671	
4.495740	0.000371	-0.003170	0.740181	-0.732524	0.217840	
2.185344	-0.000210	0.001829	0.169409	-0.097621	0.018794	
1.072975	0.000107	-0.000903	0.000786	0.834387	-0.315883	
0.487918	-0.000036	0.000234	0.002360	0.510397	-0.340603	
0.124402	0.000015	-0.000106	-0.000413	0.025378	0.256810	
0.063312	-0.000011	0.000077	0.000308	-0.010118	0.620590	
0.027945	0.000003	-0.000021	-0.000084	0.002150	0.311897	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-100.406010	-16.699495	-2.041151		-10.444555	-0.543897
50870.17	0.000043	-0.000019	0.000007	1707.052	0.000209	-0.000062
12040.90	0.000379	-0.000166	0.000062	515.9245	0.002021	-0.000598
3910.758	0.002194	-0.000962	0.000359	201.2244	0.011617	-0.003449
1496.782	0.009733	-0.004303	0.001610	89.22222	0.045292	-0.013551
635.7903	0.034826	-0.015637	0.005860	42.49527	0.127651	-0.038674
290.5279	0.100496	-0.046619	0.017588	21.19390	0.254686	-0.077307
139.9684	0.222878	-0.108461	0.041202	10.75647	0.350397	-0.101373
69.93526	0.348144	-0.180915	0.069800	5.504799	0.307328	-0.070735
35.87106	0.318770	-0.153313	0.057486	2.788770	0.132697	0.091100
18.49267	0.129551	0.114659	-0.062557	1.347391	0.019481	0.321758
9.416487	0.015253	0.461306	-0.240749	0.625164	0.000572	0.420417
4.833441	0.001123	0.442733	-0.269434	0.277230	0.000097	0.301089
2.417681	-0.000150	0.121250	0.131884	0.112819	-0.000015	0.091012
1.193222	0.000064	0.004845	0.547956			
0.560377	-0.000055	0.001300	0.432747			
0.236287	0.000008	-0.000163	0.082403			

Table XIX. Tc 6S ($24s16p13d$) basis set. Energy(E_H) = -4204.788442

Exponent	s space				
	1s	2s	3s	4s	5s
	-758.042920	-109.069670	-20.131712	-3.152082	-0.231191
58025010.	0.000001	0.000000	0.000000	0.000000	0.000000
8686877.	0.000009	-0.000003	0.000001	-0.000001	0.000000
1976901.	0.000049	-0.000016	0.000007	-0.000003	0.000001
560009.4	0.000206	-0.000066	0.000028	-0.000011	0.000003
182723.9	0.000752	-0.000241	0.000102	-0.000041	0.000010
65976.76	0.002454	-0.000787	0.000333	-0.000133	0.000034
25737.97	0.007318	-0.002360	0.001002	-0.000400	0.000102
10678.52	0.020110	-0.006553	0.002784	-0.001113	0.000285
4660.199	0.050633	-0.016949	0.007234	-0.002891	0.000735
2121.655	0.114135	-0.040216	0.017265	-0.006917	0.001771
1001.146	0.218087	-0.085639	0.037372	-0.014991	0.003808
487.1659	0.317715	-0.152166	0.068236	-0.027581	0.007089
243.2587	0.288363	-0.193652	0.091886	-0.037374	0.009454
123.6392	0.117042	-0.065620	0.033311	-0.014068	0.003842
61.03313	0.011257	0.338170	-0.216351	0.094090	-0.024820
31.60845	0.000200	0.559775	-0.513584	0.235980	-0.060398
16.38781	-0.000054	0.259651	-0.242465	0.121341	-0.034216
7.852069	-0.000018	0.025846	0.586226	-0.370038	0.106017
4.030749	-0.000038	-0.000227	0.663959	-0.712398	0.205841
1.884533	0.000019	0.000321	0.110761	0.093181	-0.030623
0.955376	-0.000007	-0.000259	-0.003087	0.839982	-0.354034
0.442146	0.000003	0.000025	0.002161	0.409191	-0.271930
0.092474	-0.000001	-0.000009	-0.000195	0.010066	0.642633
0.034698	0.000000	0.000003	0.000077	-0.002446	0.542476

p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-100.405970	-16.699455	-2.041113		-10.444515	-0.543858
50826.04	0.000043	-0.000019	0.000007	1707.358	0.000209	-0.000062
12030.70	0.000380	-0.000166	0.000062	516.0062	0.002020	-0.000598
3907.522	0.002197	-0.000963	0.000360	201.2509	0.011614	-0.003449
1495.569	0.009746	-0.004308	0.001612	89.23211	0.045284	-0.013549
635.2835	0.034868	-0.015656	0.005867	42.49919	0.127640	-0.038670
290.2996	0.100601	-0.046669	0.017608	21.19516	0.254690	-0.077310
139.8577	0.223055	-0.108554	0.041238	10.75665	0.350416	-0.101379
69.87805	0.348271	-0.180995	0.069833	5.504721	0.307337	-0.070737
35.84000	0.318620	-0.153147	0.057409	2.788671	0.132691	0.091116
18.47495	0.129303	0.115194	-0.062798	1.347344	0.019477	0.321762
9.407005	0.015183	0.461685	-0.241008	0.625119	0.000573	0.420479
4.828490	0.001123	0.442332	-0.269154	0.277178	0.000096	0.301051
2.414786	-0.000152	0.120870	0.132740	0.112801	-0.000015	0.090965
1.192006	0.000065	0.004797	0.547976			
0.559948	-0.000055	0.001302	0.432261			
0.236102	0.000009	-0.000163	0.082212			

Table XX. Tc 6S ($26s16p13d$) basis set. Energy(E_H) = -4204.788509

s space						
Exponent	1s	2s	3s	4s	5s	
	-758.042980	-109.069720	-20.131767	-3.152132	-0.231243	
84717400.	0.000001	0.000000	0.000000	0.000000	0.000000	
12749010.	0.000006	-0.000002	0.000001	0.000000	0.000000	
2917781.	0.000030	-0.000010	0.000004	-0.000002	0.000000	
830840.3	0.000125	-0.000040	0.000017	-0.000007	0.000002	
272490.1	0.000454	-0.000145	0.000062	-0.000025	0.000006	
98903.83	0.001475	-0.000472	0.000200	-0.000080	0.000020	
38781.17	0.004387	-0.001410	0.000598	-0.000239	0.000061	
16169.06	0.012085	-0.003914	0.001662	-0.000664	0.000169	
7089.197	0.030864	-0.010165	0.004326	-0.001731	0.000442	
3241.927	0.072146	-0.024609	0.010525	-0.004206	0.001072	
1536.373	0.149380	-0.054639	0.023591	-0.009468	0.002419	
750.4791	0.256313	-0.107324	0.047234	-0.018962	0.004833	
375.9836	0.320759	-0.171622	0.078333	-0.031806	0.008150	
191.6620	0.232924	-0.174410	0.084707	-0.034504	0.008786	
97.45771	0.064654	0.032806	-0.018477	0.007180	-0.001729	
51.24605	0.001871	0.431793	-0.300557	0.133324	-0.034772	
27.15478	0.001231	0.507281	-0.504150	0.233771	-0.060572	
14.31612	-0.000625	0.181455	-0.111509	0.059882	-0.017066	
7.271892	0.000287	0.013542	0.642859	-0.427862	0.120810	
3.814763	-0.000202	0.001289	0.593407	-0.667027	0.197975	
1.841266	0.000106	-0.000368	0.093967	0.147961	-0.058810	
0.936965	-0.000051	0.000052	-0.001541	0.818787	-0.330239	
0.444117	0.000019	-0.000067	0.001956	0.397594	-0.290386	
0.120630	-0.000007	0.000017	-0.000320	0.015881	0.329389	
0.057331	0.000005	-0.000012	0.000222	-0.005433	0.621218	
0.025934	-0.000001	0.000003	-0.000065	0.001268	0.248625	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-100.406020	-16.699507	-2.041161		-10.444567	-0.543908
50536.21	0.000043	-0.000019	0.000007	1703.907	0.000210	-0.000062
11967.00	0.000383	-0.000167	0.000063	514.9879	0.002029	-0.000600
3888.220	0.002215	-0.000971	0.000363	200.8760	0.011654	-0.003461
1488.616	0.009818	-0.004341	0.001624	89.07686	0.045408	-0.013586
632.4927	0.035095	-0.015760	0.005906	42.43043	0.127891	-0.038748
289.0989	0.101126	-0.046924	0.017705	21.16285	0.254963	-0.077387
139.3134	0.223826	-0.108962	0.041393	10.74104	0.350476	-0.101383
69.62306	0.348632	-0.181247	0.069941	5.497212	0.307023	-0.070549
35.71634	0.317827	-0.152383	0.057066	2.785001	0.132342	0.091515
18.41228	0.128350	0.117019	-0.063614	1.345691	0.019385	0.322013
9.377044	0.014955	0.462662	-0.241717	0.624435	0.000572	0.420325
4.814127	0.001123	0.441008	-0.268244	0.276924	0.000095	0.300761
2.407017	-0.000157	0.119808	0.135078	0.112710	-0.000015	0.090793
1.188443	0.000067	0.004679	0.548391			
0.558457	-0.000056	0.001302	0.430692			
0.235510	0.000009	-0.000164	0.081577			

Table XXI. Ru $5D$ ($23s15p12d$) basis set. Energy(E_H) = -4441.486610

Exponent	s space				
	1s	2s	3s	4s	5s
	-795.670620	-115.323250	-21.578745	-3.411188	-0.239760
38362550.	0.000002	-0.000001	0.000000	0.000000	0.000000
5743601.	0.000016	-0.000005	0.000002	-0.000001	0.000000
1307007.	0.000087	-0.000028	0.000012	-0.000005	0.000001
370195.5	0.000366	-0.000117	0.000050	-0.000020	0.000005
120774.5	0.001334	-0.000428	0.000182	-0.000074	0.000019
43603.70	0.004344	-0.001399	0.000598	-0.000242	0.000061
17008.47	0.012877	-0.004175	0.001782	-0.000722	0.000183
7056.051	0.034843	-0.011528	0.004943	-0.002005	0.000506
3078.927	0.084895	-0.029166	0.012547	-0.005092	0.001290
1401.416	0.178389	-0.066793	0.029146	-0.011860	0.002990
661.1307	0.296559	-0.130281	0.057996	-0.023691	0.006020
321.4469	0.327982	-0.195476	0.091540	-0.037747	0.009503
159.2115	0.180552	-0.135122	0.067433	-0.028206	0.007301
74.21842	0.027101	0.235255	-0.142637	0.061866	-0.016149
38.09015	-0.001830	0.574459	-0.492563	0.228215	-0.058121
19.46406	0.001040	0.341839	-0.357298	0.177070	-0.047791
8.972665	-0.000596	0.043087	0.500012	-0.307504	0.086607
4.607321	0.000318	-0.002752	0.727455	-0.757586	0.217911
2.186535	-0.000173	0.001458	0.143438	0.001870	-0.002719
1.087507	0.000086	-0.000743	-0.001585	0.861516	-0.352152
0.493425	-0.000024	0.000152	0.002240	0.445592	-0.284780
0.099136	0.000005	-0.000033	-0.000186	0.011150	0.635793
0.036809	-0.000002	0.000013	0.000076	-0.002789	0.545546

p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-106.402430	-18.012357	-2.241298		-11.505334	-0.568830
37452.67	0.000079	-0.000035	0.000013	1293.718	0.000435	-0.000134
8867.424	0.000701	-0.000309	0.000118	390.3421	0.004107	-0.001258
2879.737	0.004018	-0.001779	0.000676	151.9384	0.022325	-0.006913
1101.303	0.017438	-0.007813	0.002983	66.80366	0.080360	-0.025007
467.0261	0.059882	-0.027426	0.010478	31.50704	0.201119	-0.063812
212.9025	0.159384	-0.076226	0.029453	15.41194	0.336386	-0.103240
102.0290	0.306809	-0.155502	0.060460	7.636638	0.362907	-0.102407
50.68028	0.371135	-0.197724	0.078338	3.783916	0.201204	0.031212
25.65502	0.218508	-0.023278	-0.001678	1.783331	0.038956	0.291575
12.76996	0.043286	0.365714	-0.187544	0.805861	0.001026	0.436544
6.425252	0.001257	0.523553	-0.320133	0.345588	0.000471	0.341011
3.234748	0.000522	0.213430	-0.018652	0.134969	-0.000038	0.115296
1.548473	-0.000205	0.017841	0.516823			
0.708724	0.000035	0.001036	0.518715			
0.295218	-0.000018	0.000007	0.122181			

Table XXII. Ru 5D ($24s16p13d$) basis set. Energy(E_H) = -4441.487026

s space						
Exponent	1s	2s	3s	4s	5s	
	-795.670760	-115.323410	-21.578908	-3.411332	-0.239866	
39310670.	0.000002	-0.000001	0.000000	0.000000	0.000000	
5885678.	0.000016	-0.000005	0.000002	-0.000001	0.000000	
1339398.	0.000084	-0.000027	0.000011	-0.000005	0.000001	
379393.3	0.000355	-0.000114	0.000049	-0.000020	0.000005	
123783.3	0.001294	-0.000415	0.000177	-0.000072	0.000018	
44692.89	0.004213	-0.001357	0.000580	-0.000235	0.000059	
17434.42	0.012493	-0.004049	0.001729	-0.000700	0.000177	
7233.200	0.033836	-0.011185	0.004796	-0.001945	0.000492	
3156.403	0.082619	-0.028337	0.012188	-0.004945	0.001251	
1436.720	0.174423	-0.065058	0.028372	-0.011548	0.002922	
677.7302	0.292747	-0.127682	0.056784	-0.023181	0.005868	
329.3980	0.329931	-0.194091	0.090688	-0.037408	0.009483	
162.9910	0.187655	-0.141759	0.070595	-0.029447	0.007482	
76.07924	0.029756	0.216284	-0.129971	0.056092	-0.014334	
39.13745	-0.001994	0.570272	-0.481101	0.222683	-0.057463	
20.01373	0.001176	0.359084	-0.380461	0.187117	-0.048938	
9.255034	-0.000682	0.048880	0.455242	-0.273278	0.073821	
4.787794	0.000384	-0.003344	0.743853	-0.753527	0.222403	
2.328582	-0.000216	0.001854	0.168783	-0.078982	0.012328	
1.149663	0.000110	-0.000922	0.000615	0.844738	-0.320474	
0.523610	-0.000036	0.000234	0.002434	0.498283	-0.329368	
0.132298	0.000015	-0.000101	-0.000409	0.023632	0.275093	
0.065744	-0.000011	0.000073	0.000303	-0.009303	0.615231	
0.029024	0.000003	-0.000020	-0.000085	0.002062	0.298207	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-106.402600	-18.012523	-2.241442		-11.505505	-0.568958
54142.82	0.000041	-0.000018	0.000007	1782.504	0.000216	-0.000066
12815.67	0.000370	-0.000163	0.000062	538.7658	0.002085	-0.000639
4162.508	0.002142	-0.000946	0.000360	210.1555	0.011982	-0.003693
1593.228	0.009509	-0.004237	0.001615	93.18781	0.046704	-0.014490
676.8489	0.034090	-0.015425	0.005887	44.39572	0.131349	-0.041353
309.3565	0.098691	-0.046124	0.017727	22.14433	0.260498	-0.081943
149.0997	0.220018	-0.107891	0.041754	11.23995	0.354700	-0.106485
74.54772	0.346357	-0.181367	0.071320	5.758339	0.301865	-0.067481
38.27596	0.321150	-0.156976	0.060085	2.919406	0.122479	0.111124
19.77165	0.133294	0.108673	-0.061338	1.420762	0.016467	0.336813
10.09082	0.016228	0.460500	-0.246751	0.661729	0.000762	0.412091
5.199727	0.001085	0.446095	-0.277183	0.293403	0.000134	0.284824
2.612360	-0.000141	0.122971	0.137784	0.119222	0.000034	0.084965
1.293023	0.000048	0.005200	0.553274			
0.608402	-0.000053	0.001330	0.427870			
0.256576	0.000007	-0.000139	0.080113			

Table XXIII. Ru 5D ($24s16p13d$) basis set. Energy(E_H) = -4441.487032

Exponent	s space				
	1s	2s	3s	4s	5s
	-795.670730	-115.323360	-21.578861	-3.411287	-0.239809
61667040.	0.000001	0.000000	0.000000	0.000000	0.000000
9234532.	0.000009	-0.000003	0.000001	-0.000001	0.000000
2101580.	0.000048	-0.000015	0.000007	-0.000003	0.000001
595293.3	0.000202	-0.000065	0.000028	-0.000011	0.000003
194224.7	0.000738	-0.000237	0.000101	-0.000041	0.000010
70126.62	0.002409	-0.000774	0.000330	-0.000134	0.000034
27356.48	0.007186	-0.002321	0.000992	-0.000402	0.000101
11350.11	0.019754	-0.006447	0.002756	-0.001118	0.000283
4953.415	0.049778	-0.016685	0.007165	-0.002904	0.000732
2255.272	0.112405	-0.039629	0.017116	-0.006958	0.001766
1064.314	0.215529	-0.084574	0.037130	-0.015109	0.003804
518.0167	0.316136	-0.150903	0.068055	-0.027915	0.007115
258.7904	0.290692	-0.194118	0.092620	-0.038216	0.009578
131.6570	0.121026	-0.071228	0.036374	-0.015592	0.004212
64.86879	0.012233	0.330102	-0.212074	0.093726	-0.024557
33.62753	0.000078	0.561257	-0.515945	0.240721	-0.061052
17.45377	0.000009	0.266867	-0.255313	0.130688	-0.036593
8.372009	-0.000051	0.027294	0.583580	-0.377898	0.107945
4.319650	-0.000019	-0.000415	0.669564	-0.730483	0.209311
2.033540	0.000009	0.000370	0.113305	0.106759	-0.035118
1.028698	-0.000001	-0.000285	-0.002637	0.845427	-0.356272
0.476428	0.000002	0.000031	0.002142	0.401812	-0.261932
0.099245	0.000000	-0.000010	-0.000184	0.009770	0.637459
0.036786	0.000000	0.000004	0.000073	-0.002349	0.545208

p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-106.402550	-18.012474	-2.241396		-11.505456	-0.568910
54116.61	0.000042	-0.000018	0.000007	1782.135	0.000216	-0.000066
12809.36	0.000370	-0.000163	0.000062	538.6504	0.002086	-0.000640
4160.430	0.002143	-0.000947	0.000360	210.1096	0.011987	-0.003695
1592.423	0.009517	-0.004240	0.001616	93.16718	0.046722	-0.014496
676.5023	0.034118	-0.015438	0.005892	44.38578	0.131389	-0.041367
309.1966	0.098761	-0.046158	0.017740	22.13893	0.260558	-0.081962
149.0203	0.220141	-0.107956	0.041779	11.23681	0.354736	-0.106493
74.50576	0.346453	-0.181427	0.071345	5.756571	0.301809	-0.067437
38.25276	0.321053	-0.156867	0.060033	2.918417	0.122399	0.111240
19.75831	0.133118	0.109055	-0.061514	1.420286	0.016444	0.336875
10.08355	0.016176	0.460786	-0.246951	0.661496	0.000762	0.412116
5.195888	0.001085	0.445806	-0.276970	0.293273	0.000133	0.284709
2.610102	-0.000142	0.122692	0.138412	0.119178	0.000035	0.084877
1.292112	0.000049	0.005163	0.553238			
0.608103	-0.000054	0.001332	0.427544			
0.256443	0.000007	-0.000139	0.079992			

Table XXIV. Ru 5D (26s16p13d) basis set. Energy(E_H) = -4441.487106

Exponent	s space					
	1s	2s	3s	4s	5s	
	-795.670800	-115.323420	-21.578924	-3.411345	-0.239868	
90011640.	0.000001	0.000000	0.000000	0.000000	0.000000	
13511130.	0.000006	-0.000002	0.000001	0.000000	0.000000	
3084114.	0.000030	-0.000009	0.000004	-0.000002	0.000000	
876844.5	0.000124	-0.000040	0.000017	-0.000007	0.000002	
287214.8	0.000451	-0.000145	0.000062	-0.000025	0.000006	
104114.5	0.001467	-0.000471	0.000201	-0.000081	0.000021	
40780.64	0.004369	-0.001407	0.000600	-0.000244	0.000062	
16990.24	0.012044	-0.003908	0.001670	-0.000676	0.000171	
7446.088	0.030769	-0.010152	0.004348	-0.001765	0.000447	
3404.497	0.071943	-0.024583	0.010579	-0.004289	0.001083	
1613.411	0.149004	-0.054599	0.023721	-0.009659	0.002447	
788.2406	0.255827	-0.107277	0.047516	-0.019353	0.004889	
395.0232	0.320623	-0.171755	0.078900	-0.032514	0.008261	
201.4367	0.233675	-0.175033	0.085603	-0.035386	0.008930	
102.4019	0.065236	0.031511	-0.017977	0.007051	-0.001668	
53.99434	0.001797	0.429756	-0.301481	0.136000	-0.035205	
28.66852	0.001306	0.507637	-0.507737	0.239334	-0.061479	
15.15799	-0.000673	0.183854	-0.117094	0.064784	-0.018386	
7.729671	0.000319	0.013988	0.645142	-0.441821	0.124331	
4.077477	-0.000221	0.001231	0.594929	-0.680333	0.200337	
1.985186	0.000116	-0.000364	0.095441	0.164368	-0.064423	
1.008129	-0.000055	0.000040	-0.001020	0.823574	-0.332002	
0.478111	0.000020	-0.000064	0.001899	0.389703	-0.280727	
0.129500	-0.000007	0.000015	-0.000287	0.015205	0.332433	
0.060575	0.000005	-0.000010	0.000199	-0.005093	0.619936	
0.027179	-0.000001	0.000003	-0.000059	0.001206	0.245061	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-106.402610	-18.012534	-2.241451		-11.505516	-0.568967
53964.10	0.000042	-0.000018	0.000007	1783.114	0.000215	-0.000066
12777.14	0.000372	-0.000164	0.000062	539.0008	0.002083	-0.000639
4151.208	0.002151	-0.000951	0.000361	210.2526	0.011971	-0.003690
1589.315	0.009546	-0.004253	0.001621	93.23163	0.046668	-0.014479
675.3326	0.034201	-0.015476	0.005907	44.41613	0.131274	-0.041330
308.7154	0.098949	-0.046250	0.017776	22.15367	0.260432	-0.081924
148.8057	0.220424	-0.108107	0.041838	11.24415	0.354701	-0.106489
74.40483	0.346600	-0.181529	0.071389	5.760238	0.301956	-0.067536
38.20322	0.320773	-0.156591	0.059906	2.920268	0.122560	0.111033
19.73278	0.132754	0.109746	-0.061830	1.421136	0.016483	0.336772
10.07167	0.016082	0.461139	-0.247215	0.661871	0.000762	0.412151
5.190393	0.001087	0.445301	-0.276612	0.293433	0.000134	0.284893
2.607285	-0.000145	0.122317	0.139204	0.119222	0.000034	0.084968
1.290891	0.000050	0.005124	0.553308			
0.607645	-0.000054	0.001332	0.427015			
0.256316	0.000007	-0.000139	0.079851			

Table XXV. Rh $^4F(23s15p12d)$ basis set. Energy(E_H) = -4685.800406

Exponent	s space				
	1s	2s	3s	4s	5s
	-834.208960	-121.740940	-23.057109	-3.668316	-0.247022
24588200.	0.000004	-0.000001	0.000001	0.000000	0.000000
3681650.	0.000030	-0.000010	0.000004	-0.000002	0.000000
837835.0	0.000160	-0.000051	0.000022	-0.000009	0.000002
237317.2	0.000675	-0.000217	0.000093	-0.000038	0.000010
77424.54	0.002455	-0.000790	0.000339	-0.000139	0.000035
27951.95	0.007958	-0.002574	0.001105	-0.000453	0.000113
10902.02	0.023323	-0.007648	0.003294	-0.001354	0.000338
4521.552	0.061548	-0.020774	0.008966	-0.003677	0.000917
1971.617	0.141791	-0.051120	0.022314	-0.009199	0.002299
895.9301	0.265711	-0.109250	0.048450	-0.019961	0.004977
420.9983	0.349196	-0.186432	0.086308	-0.036036	0.009033
201.9002	0.244735	-0.184253	0.090630	-0.037933	0.009454
93.05059	0.052082	0.109688	-0.062765	0.026436	-0.006517
47.45681	-0.002903	0.547771	-0.429865	0.200344	-0.051256
23.85193	0.002084	0.448602	-0.481633	0.235076	-0.059882
10.88915	-0.001232	0.078838	0.298447	-0.166090	0.042166
5.717135	0.000780	-0.006750	0.792697	-0.755982	0.221094
2.892500	-0.000417	0.003506	0.253013	-0.239568	0.059356
1.334705	0.000185	-0.001430	0.010580	0.827098	-0.301215
0.598085	-0.000066	0.000416	0.001439	0.566276	-0.350658
0.154856	0.000029	-0.000190	-0.000032	0.031850	0.165401
0.079312	-0.000021	0.000133	0.000043	-0.011949	0.638566
0.032820	0.000005	-0.000034	-0.000012	0.002293	0.374292

p space				d space		
Exponent	2p	3p	4p	Exponent	3d	4d
	-112.561970	-19.355750	-2.440736		-12.595757	-0.611190
39643.90	0.000078	-0.000034	0.000013	1359.439	0.000441	-0.000140
9386.159	0.000689	-0.000306	0.000119	410.2416	0.004166	-0.001318
3048.253	0.003953	-0.001763	0.000680	159.7152	0.022669	-0.007252
1165.832	0.017171	-0.007750	0.003006	70.25153	0.081688	-0.026292
494.4660	0.059072	-0.027253	0.010580	33.15638	0.204167	-0.066966
225.4682	0.157711	-0.075979	0.029826	16.23202	0.340171	-0.107980
108.1013	0.304994	-0.155751	0.061563	8.060572	0.362000	-0.104364
53.73074	0.371496	-0.199601	0.080366	4.009057	0.193795	0.041860
27.22384	0.221190	-0.026784	-0.000247	1.905150	0.035938	0.305245
13.57142	0.044514	0.365088	-0.191738	0.865104	0.001173	0.434373
6.850808	0.001237	0.525825	-0.328482	0.371991	0.000474	0.328758
3.458486	0.000534	0.213030	-0.013247	0.145507	0.000010	0.108889
1.665213	-0.000226	0.017820	0.523886			
0.764061	0.000036	0.001158	0.513749			
0.318823	-0.000020	0.000018	0.119243			

Table XXVI. Rh 4F ($23s15p12d$) basis set. Energy(E_H) = -4685.800470

s space						
Exponent	1s	2s	3s	4s	5s	
	-834.208960	-121.740900	-23.057060	-3.668277	-0.246962	
40450100.	0.000002	-0.000001	0.000000	0.000000	0.000000	
6056216.	0.000016	-0.000005	0.000002	-0.000001	0.000000	
1378203.	0.000086	-0.000028	0.000012	-0.000005	0.000001	
390385.6	0.000363	-0.000116	0.000050	-0.000021	0.000005	
127369.4	0.001321	-0.000424	0.000182	-0.000075	0.000019	
45987.20	0.004301	-0.001388	0.000596	-0.000245	0.000061	
17939.05	0.012749	-0.004140	0.001778	-0.000730	0.000182	
7442.428	0.034509	-0.011435	0.004932	-0.002025	0.000504	
3247.660	0.084143	-0.028946	0.012525	-0.005147	0.001288	
1478.285	0.177092	-0.066357	0.029124	-0.011998	0.002984	
697.4219	0.295342	-0.129722	0.058082	-0.024031	0.006028	
339.0931	0.328651	-0.195491	0.092074	-0.038436	0.009547	
167.9448	0.182832	-0.137474	0.069029	-0.029281	0.007486	
78.36688	0.027918	0.230337	-0.140546	0.061872	-0.015969	
40.26990	-0.001890	0.573819	-0.494194	0.232003	-0.058292	
20.59616	0.001078	0.346525	-0.365797	0.184831	-0.049347	
9.514624	-0.000621	0.044360	0.498997	-0.314580	0.087899	
4.910723	0.000335	-0.002950	0.731012	-0.774582	0.220033	
2.339642	-0.000180	0.001496	0.144735	0.017575	-0.008202	
1.163437	0.000089	-0.000759	-0.001285	0.866327	-0.351345	
0.528269	-0.000025	0.000155	0.002240	0.437225	-0.274468	
0.105181	0.000005	-0.000033	-0.000179	0.010689	0.630520	
0.038627	-0.000002	0.000013	0.000073	-0.002669	0.547657	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-112.561920	-19.355701	-2.440692		-12.595708	-0.611143
39626.14	0.000078	-0.000034	0.000013	1359.322	0.000441	-0.000140
9381.996	0.000690	-0.000307	0.000119	410.2025	0.004167	-0.001319
3046.891	0.003956	-0.001764	0.000681	159.6994	0.022674	-0.007253
1165.300	0.017184	-0.007756	0.003008	70.24408	0.081702	-0.026297
494.2333	0.059115	-0.027273	0.010588	33.15241	0.204196	-0.066976
225.3572	0.157809	-0.076029	0.029845	16.22996	0.340190	-0.107987
108.0450	0.305119	-0.155822	0.061593	8.059619	0.361981	-0.104354
53.70177	0.371479	-0.199587	0.080358	4.008629	0.193758	0.041892
27.20879	0.221015	-0.026522	-0.000367	1.905018	0.035927	0.305258
13.56379	0.044429	0.365389	-0.191912	0.865022	0.001174	0.434417
6.847197	0.001234	0.525706	-0.328431	0.371940	0.000473	0.328707
3.456667	0.000532	0.212761	-0.012908	0.145497	0.000010	0.108856
1.664848	-0.000225	0.017775	0.523828			
0.764012	0.000036	0.001163	0.513681			
0.318803	-0.000019	0.000017	0.119217			

Table XXVII. Rh 4F ($24s16p13d$) basis set. Energy(E_H) = -4685.800914

Exponent	s space				
	1s	2s	3s	4s	5s
	-834.209110	-121.741060	-23.057235	-3.668432	-0.247076
41391280.	0.000002	-0.000001	0.000000	0.000000	0.000000
6197630.	0.000016	-0.000005	0.000002	-0.000001	0.000000
1410481.	0.000083	-0.000027	0.000011	-0.000005	0.000001
399558.9	0.000352	-0.000113	0.000049	-0.000020	0.000005
130372.2	0.001283	-0.000412	0.000177	-0.000073	0.000018
47074.82	0.004177	-0.001348	0.000579	-0.000238	0.000059
18364.55	0.012388	-0.004022	0.001727	-0.000709	0.000177
7619.409	0.033562	-0.011113	0.004792	-0.001968	0.000491
3325.041	0.082002	-0.028167	0.012185	-0.005006	0.001250
1513.517	0.173358	-0.064724	0.028391	-0.011698	0.002920
713.9626	0.291732	-0.127271	0.056933	-0.023541	0.005882
347.0005	0.330436	-0.194157	0.091252	-0.038103	0.009530
171.6982	0.189527	-0.143663	0.071992	-0.030458	0.007645
80.22838	0.030466	0.212407	-0.128522	0.056317	-0.014225
41.31465	-0.002035	0.569701	-0.483199	0.226615	-0.057698
21.14202	0.001205	0.362818	-0.387612	0.194383	-0.050318
9.793576	-0.000701	0.049925	0.456429	-0.281222	0.075399
5.089268	0.000398	-0.003527	0.747014	-0.772017	0.225118
2.477982	-0.000222	0.001879	0.168338	-0.060347	0.005643
1.226436	0.000112	-0.000935	0.000618	0.852846	-0.321447
0.558858	-0.000037	0.000234	0.002466	0.486856	-0.317810
0.139417	0.000014	-0.000097	-0.000397	0.022047	0.286754
0.068069	-0.000010	0.000069	0.000295	-0.008671	0.610391
0.030000	0.000003	-0.000020	-0.000085	0.001980	0.289204

Exponent	p space			d space		
	2p	3p	4p	Exponent	3d	4d
	-112.562100	-19.355879	-2.440847		-12.595891	-0.611285
57553.11	0.000040	-0.000018	0.000007	1876.497	0.000218	-0.000069
13622.76	0.000361	-0.000160	0.000062	567.2167	0.002106	-0.000667
4424.645	0.002091	-0.000931	0.000359	221.2820	0.012120	-0.003862
1693.610	0.009294	-0.004171	0.001615	98.14694	0.047327	-0.015170
719.5669	0.033381	-0.015214	0.005899	46.78383	0.133179	-0.043389
328.9400	0.096943	-0.045624	0.017816	23.34980	0.263772	-0.085722
158.5950	0.217223	-0.107284	0.042188	11.86249	0.357493	-0.111030
79.34420	0.344558	-0.181717	0.072636	6.088411	0.298427	-0.065275
40.77729	0.323419	-0.160487	0.062544	3.091430	0.116193	0.126089
21.10261	0.136996	0.102719	-0.059873	1.513639	0.014752	0.347017
10.79311	0.017223	0.459475	-0.251944	0.708371	0.000895	0.405605
5.581729	0.001048	0.449418	-0.284257	0.315016	0.000162	0.272422
2.815848	-0.000131	0.124861	0.142415	0.128250	0.000063	0.079606
1.396871	0.000032	0.005598	0.557041			
0.658205	-0.000052	0.001362	0.424381			
0.277963	0.000005	-0.000116	0.078759			

Table XXVIII. Rh $4F$ ($24s16p13d$) basis set. Energy(E_H) = -4685.800916

Exponent	s space				
	1s	2s	3s	4s	5s
	-834.209070	-121.741010	-23.057181	-3.668379	-0.247012
65362240.	0.000001	0.000000	0.000000	0.000000	0.000000
9787537.	0.000009	-0.000003	0.000001	-0.000001	0.000000
2227343.	0.000047	-0.000015	0.000006	-0.000003	0.000001
630920.8	0.000199	-0.000064	0.000027	-0.000011	0.000003
205860.1	0.000726	-0.000233	0.000100	-0.000041	0.000010
74332.85	0.002370	-0.000762	0.000327	-0.000134	0.000034
28999.16	0.007069	-0.002288	0.000983	-0.000403	0.000100
12032.29	0.019440	-0.006355	0.002732	-0.001122	0.000281
5251.391	0.049023	-0.016453	0.007106	-0.002916	0.000725
2391.090	0.110872	-0.039114	0.016990	-0.006994	0.001752
1128.527	0.213248	-0.083638	0.036929	-0.015213	0.003779
549.3711	0.314691	-0.149798	0.067921	-0.028215	0.007098
274.5580	0.292736	-0.194519	0.093309	-0.038977	0.009638
139.7693	0.124600	-0.076142	0.039097	-0.016978	0.004516
68.77542	0.013121	0.322820	-0.208270	0.093347	-0.024172
35.69017	-0.000025	0.562271	-0.518063	0.244929	-0.061292
18.54742	0.000063	0.273497	-0.267003	0.139389	-0.038543
8.902831	-0.000079	0.028716	0.581607	-0.385546	0.109182
4.615570	-0.000002	-0.000634	0.674267	-0.746117	0.211047
2.186626	0.000001	0.000432	0.115527	0.119819	-0.039455
1.102814	0.000003	-0.000315	-0.002157	0.849518	-0.354749
0.510595	0.000000	0.000039	0.002110	0.395260	-0.252681
0.105257	0.000000	-0.000011	-0.000172	0.009402	0.632216
0.038598	0.000000	0.000004	0.000068	-0.002261	0.547116

p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-112.562040	-19.355822	-2.440794		-12.595835	-0.611229
57530.00	0.000041	-0.000018	0.000007	1875.259	0.000218	-0.000069
13616.39	0.000361	-0.000160	0.000062	566.8808	0.002109	-0.000668
4422.374	0.002093	-0.000932	0.000360	221.1622	0.012132	-0.003866
1692.686	0.009303	-0.004175	0.001616	98.09731	0.047365	-0.015182
719.1553	0.033412	-0.015229	0.005904	46.76144	0.133260	-0.043416
328.7443	0.097025	-0.045664	0.017832	23.33859	0.263876	-0.085755
158.4952	0.217373	-0.107363	0.042219	11.85644	0.357541	-0.111041
79.29024	0.344683	-0.181795	0.072670	6.085112	0.298317	-0.065184
40.74685	0.323312	-0.160359	0.062482	3.089591	0.116054	0.126296
21.08477	0.136776	0.103196	-0.060096	1.512768	0.014715	0.347105
10.78344	0.017153	0.459843	-0.252207	0.707977	0.000896	0.405580
5.576591	0.001049	0.449061	-0.283979	0.314828	0.000161	0.272249
2.812798	-0.000133	0.124507	0.143216	0.128190	0.000063	0.079502
1.395610	0.000033	0.005551	0.557014			
0.657768	-0.000053	0.001365	0.423947			
0.277777	0.000005	-0.000117	0.078600			

Table XXIX. Rh $^4F(26s16p13d)$ basis set. Energy(E_H) = -4685.800996

Exponent	s space					
	1s	2s	3s	4s	5s	
	-834.209140	-121.741080	-23.057251	-3.668445	-0.247077	
94432490.	0.000001	0.000000	0.000000	0.000000	0.000000	
14219000.	0.000006	-0.000002	0.000001	0.000000	0.000000	
3255731.	0.000029	-0.000009	0.000004	-0.000002	0.000000	
927140.0	0.000123	-0.000039	0.000017	-0.000007	0.000002	
304014.7	0.000444	-0.000143	0.000061	-0.000025	0.000006	
110321.6	0.001443	-0.000464	0.000199	-0.000082	0.000020	
43248.00	0.004293	-0.001385	0.000594	-0.000244	0.000061	
18027.95	0.011832	-0.003846	0.001653	-0.000678	0.000169	
7903.690	0.030235	-0.009990	0.004303	-0.001768	0.000442	
3614.721	0.070760	-0.024203	0.010476	-0.004300	0.001072	
1713.474	0.146875	-0.053816	0.023512	-0.009695	0.002424	
837.3163	0.253329	-0.106059	0.047240	-0.019480	0.004856	
419.6971	0.320341	-0.170773	0.078852	-0.032907	0.008252	
214.1231	0.237132	-0.177019	0.087025	-0.036425	0.009071	
109.1601	0.068218	0.023661	-0.013764	0.005310	-0.001204	
57.45359	0.002277	0.423071	-0.297321	0.135940	-0.034749	
30.50628	0.001260	0.512151	-0.512983	0.245134	-0.062166	
16.15875	-0.000650	0.190471	-0.130615	0.073551	-0.020521	
8.239730	0.000307	0.015105	0.644667	-0.451481	0.125807	
4.362340	-0.000216	0.001076	0.600597	-0.694770	0.202046	
2.136374	0.000113	-0.000315	0.097779	0.176061	-0.068278	
1.081843	-0.000053	0.000008	-0.000594	0.828058	-0.330443	
0.512433	0.000019	-0.000054	0.001868	0.383877	-0.271994	
0.137537	-0.000006	0.000011	-0.000266	0.014571	0.331867	
0.063670	0.000004	-0.000008	0.000185	-0.004866	0.617221	
0.028366	-0.000001	0.000002	-0.000055	0.001163	0.245257	
	p space			d space		
Exponent	2p	3p	4p	Exponent	3d	4d
	-112.562110	-19.355890	-2.440857		-12.595902	-0.611294
57298.74	0.000041	-0.000018	0.000007	1872.137	0.000219	-0.000069
13565.13	0.000363	-0.000161	0.000062	566.0036	0.002116	-0.000670
4406.598	0.002105	-0.000937	0.000362	220.8417	0.012165	-0.003877
1686.911	0.009354	-0.004198	0.001626	97.96214	0.047470	-0.015216
716.7974	0.033577	-0.015305	0.005934	46.70007	0.133477	-0.043489
327.7063	0.097425	-0.045861	0.017910	23.30930	0.264105	-0.085823
158.0112	0.218003	-0.107701	0.042352	11.84247	0.357557	-0.111034
79.05636	0.345046	-0.182041	0.072777	6.078660	0.298016	-0.064985
40.63015	0.322724	-0.159776	0.062208	3.086637	0.115798	0.126593
21.02420	0.135958	0.104766	-0.060828	1.511611	0.014665	0.347140
10.75402	0.016936	0.460784	-0.252902	0.707639	0.000895	0.405351
5.562181	0.001049	0.447920	-0.283137	0.314777	0.000161	0.272142
2.804901	-0.000139	0.123551	0.145398	0.128183	0.000063	0.079492
1.391790	0.000035	0.005442	0.557398			
0.656105	-0.000053	0.001363	0.422478			
0.277099	0.000006	-0.000118	0.078009			

Table XXX. Pd $^3F(23s15p12d)$ basis set. Energy(E_H) = -4937.782145

Exponent	s space				
	1s	2s	3s	4s	5s
	-873.662920	-128.327810	-24.571739	-3.927291	-0.253560
25575060.	0.000004	-0.000001	0.000001	0.000000	0.000000
3829463.	0.000031	-0.000010	0.000004	-0.000002	0.000000
871502.6	0.000161	-0.000052	0.000022	-0.000009	0.000002
246862.5	0.000679	-0.000218	0.000094	-0.000039	0.000010
80541.23	0.002469	-0.000796	0.000344	-0.000143	0.000035
29078.00	0.008003	-0.002593	0.001119	-0.000464	0.000114
11341.53	0.023452	-0.007705	0.003337	-0.001386	0.000341
4703.971	0.061872	-0.020924	0.009080	-0.003767	0.000925
2051.237	0.142444	-0.051482	0.022601	-0.009418	0.002318
932.1692	0.266572	-0.109942	0.049041	-0.020439	0.005024
438.0734	0.349310	-0.187330	0.087282	-0.036832	0.009091
210.1136	0.243491	-0.183805	0.091021	-0.038600	0.009497
96.70691	0.051210	0.114702	-0.066335	0.028506	-0.006979
49.35331	-0.002986	0.551118	-0.438214	0.206663	-0.052022
24.81427	0.002074	0.444192	-0.480196	0.238950	-0.060265
11.29779	-0.001227	0.076093	0.323639	-0.188016	0.047989
5.937500	0.000777	-0.006885	0.794864	-0.784035	0.225947
2.979345	-0.000418	0.003444	0.234351	-0.194697	0.044798
1.401431	0.000188	-0.001447	0.007995	0.847530	-0.307463
0.627442	-0.000064	0.000401	0.001827	0.541757	-0.333865
0.154299	0.000027	-0.000174	-0.000159	0.027666	0.220394
0.077891	-0.000020	0.000126	0.000133	-0.011204	0.616492
0.033016	0.000005	-0.000034	-0.000036	0.002339	0.341089

Exponent	p space			Exponent	d space	
	2p	3p	4p		3d	4d
	-118.889610	-20.734559	-2.642679		-13.720575	-0.657193
41889.99	0.000076	-0.000034	0.000013	1427.756	0.000446	-0.000145
9918.000	0.000678	-0.000304	0.000119	430.9161	0.004216	-0.001374
3220.979	0.003893	-0.001748	0.000684	167.7932	0.022969	-0.007560
1231.930	0.016927	-0.007693	0.003026	73.83290	0.082871	-0.027482
522.5530	0.058338	-0.027099	0.010670	34.86864	0.206939	-0.069886
238.3204	0.156201	-0.075773	0.030163	17.08266	0.343668	-0.112427
114.3077	0.303364	-0.156027	0.062579	8.499527	0.361059	-0.105801
56.84749	0.371807	-0.201366	0.082239	4.240431	0.187013	0.052166
28.82677	0.223602	-0.029928	0.001076	2.030714	0.033329	0.316646
14.39071	0.045625	0.364730	-0.195736	0.926612	0.001353	0.431784
7.287032	0.001214	0.527818	-0.336040	0.399703	0.000496	0.317952
3.687892	0.000543	0.212514	-0.007703	0.156696	0.000057	0.103181
1.784669	-0.000246	0.017803	0.529767			
0.820709	0.000037	0.001273	0.509169			
0.343083	-0.000021	0.000029	0.116832			

Table XXXI. Pd 3F ($23s15p12d$) basis set. Energy(E_H) = -4937.782208

s space						
Exponent	1s	2s	3s	4s	5s	
	-873.662900	-128.327760	-24.571682	-3.927240	-0.253491	
42606480.	0.000002	-0.000001	0.000000	0.000000	0.000000	
6379178.	0.000016	-0.000005	0.000002	-0.000001	0.000000	
1451725.	0.000085	-0.000027	0.000012	-0.000005	0.000001	
411219.4	0.000359	-0.000116	0.000050	-0.000021	0.000005	
134169.4	0.001308	-0.000421	0.000182	-0.000075	0.000019	
48443.38	0.004259	-0.001377	0.000595	-0.000247	0.000061	
18897.54	0.012626	-0.004107	0.001773	-0.000736	0.000181	
7840.218	0.034188	-0.011346	0.004920	-0.002042	0.000501	
3421.303	0.083423	-0.028735	0.012502	-0.005195	0.001281	
1557.355	0.175852	-0.065940	0.029099	-0.012118	0.002969	
734.7338	0.294174	-0.129187	0.058159	-0.024335	0.006016	
357.2266	0.329277	-0.195501	0.092579	-0.039068	0.009559	
176.9156	0.185015	-0.139702	0.070556	-0.030301	0.007637	
82.62830	0.028714	0.225662	-0.138532	0.061798	-0.015741	
42.50979	-0.001948	0.573164	-0.495718	0.235451	-0.058281	
21.76017	0.001116	0.350977	-0.373945	0.192244	-0.050667	
10.07313	-0.000645	0.045588	0.498043	-0.321207	0.088836	
5.224125	0.000351	-0.003141	0.734214	-0.789703	0.221157	
2.499190	-0.000187	0.001530	0.146118	0.031899	-0.013187	
1.241038	0.000091	-0.000771	-0.000910	0.870176	-0.348783	
0.563547	-0.000025	0.000156	0.002225	0.429884	-0.265163	
0.110894	0.000005	-0.000033	-0.000170	0.010244	0.625446	
0.040320	-0.000002	0.000013	0.000069	-0.002564	0.549386	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-118.889550	-20.734499	-2.642625		-13.720516	-0.657135
41868.28	0.000076	-0.000034	0.000013	1427.627	0.000446	-0.000146
9912.706	0.000679	-0.000304	0.000119	430.8802	0.004217	-0.001374
3219.271	0.003896	-0.001750	0.000685	167.7792	0.022973	-0.007562
1231.297	0.016941	-0.007699	0.003028	73.82588	0.082885	-0.027487
522.2931	0.058380	-0.027119	0.010678	34.86466	0.206969	-0.069897
238.2033	0.156293	-0.075820	0.030182	17.08049	0.343690	-0.112435
114.2512	0.303472	-0.156091	0.062606	8.498462	0.361041	-0.105789
56.81953	0.371786	-0.201348	0.082230	4.239912	0.186974	0.052204
28.81266	0.223441	-0.029700	0.000970	2.030534	0.033315	0.316664
14.38412	0.045549	0.364967	-0.195877	0.926507	0.001354	0.431820
7.284053	0.001213	0.527710	-0.335987	0.399648	0.000495	0.317893
3.686453	0.000541	0.212308	-0.007448	0.156687	0.000057	0.103153
1.784433	-0.000245	0.017771	0.529693			
0.820696	0.000037	0.001277	0.509146			
0.343069	-0.000021	0.000028	0.116817			

Table XXXII. Pd 3F (24s16p13d) basis set. Energy(E_H) = -4937.782679

s space						
Exponent	1s	2s	3s	4s	5s	
	-873.663060	-128.327940	-24.571866	-3.927404	-0.253612	
43587320.	0.000002	-0.000001	0.000000	0.000000	0.000000	
6525927.	0.000016	-0.000005	0.000002	-0.000001	0.000000	
1485090.	0.000083	-0.000027	0.000011	-0.000005	0.000001	
420662.9	0.000349	-0.000112	0.000048	-0.000020	0.000005	
137248.7	0.001272	-0.000409	0.000176	-0.000073	0.000018	
49554.54	0.004141	-0.001338	0.000578	-0.000240	0.000059	
19330.74	0.012282	-0.003994	0.001725	-0.000715	0.000176	
8019.808	0.033286	-0.011038	0.004786	-0.001987	0.000488	
3499.581	0.081388	-0.027993	0.012177	-0.005059	0.001244	
1592.892	0.172302	-0.064387	0.028398	-0.011828	0.002909	
751.3731	0.290726	-0.126854	0.057059	-0.023861	0.005875	
365.1616	0.330931	-0.194206	0.091778	-0.038739	0.009545	
180.6765	0.191391	-0.145530	0.073358	-0.031426	0.007778	
84.50333	0.031185	0.208572	-0.127025	0.056421	-0.014058	
43.55903	-0.002080	0.569108	-0.485103	0.230173	-0.057743	
22.30549	0.001236	0.366490	-0.394667	0.201403	-0.051485	
10.35104	-0.000722	0.050960	0.457257	-0.288553	0.076586	
5.401995	0.000412	-0.003698	0.749952	-0.788436	0.226774	
2.634217	-0.000228	0.001899	0.168282	-0.043155	-0.000577	
1.304909	0.000114	-0.000944	0.000721	0.859127	-0.320329	
0.594685	-0.000037	0.000233	0.002482	0.476823	-0.307210	
0.146744	0.000014	-0.000094	-0.000386	0.020752	0.291442	
0.070724	-0.000010	0.000067	0.000286	-0.008154	0.606671	
0.031045	0.000003	-0.000020	-0.000083	0.001896	0.285595	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-118.889740	-20.734687	-2.642789		-13.720710	-0.657288
61046.72	0.000040	-0.000018	0.000007	1977.157	0.000218	-0.000071
14449.39	0.000353	-0.000158	0.000062	597.7286	0.002116	-0.000689
4693.096	0.002045	-0.000917	0.000359	233.2300	0.012193	-0.004001
1796.403	0.009100	-0.004112	0.001614	103.4830	0.047715	-0.015741
763.3101	0.032740	-0.015025	0.005907	49.35980	0.134429	-0.045134
348.9947	0.095357	-0.045175	0.017891	24.65503	0.266199	-0.089056
168.3200	0.214667	-0.106740	0.042570	12.54054	0.359664	-0.115115
84.25809	0.342865	-0.182051	0.073832	6.450127	0.295580	-0.063228
43.34063	0.325434	-0.163697	0.064818	3.280952	0.111416	0.138855
22.46687	0.140416	0.097283	-0.058450	1.613914	0.013569	0.354971
11.51393	0.018167	0.458584	-0.256748	0.758417	0.001027	0.399823
5.974577	0.001012	0.452357	-0.290586	0.338277	0.000214	0.262050
3.025301	-0.000123	0.126571	0.146749	0.137994	0.000089	0.075084
1.503490	0.000016	0.005987	0.560067			
0.709283	-0.000051	0.001395	0.421360			
0.300020	0.000004	-0.000095	0.077721			

Table XXXIII. Pd 3F ($24s16p13d$) basis set. Energy(E_H) = -4937.782677

s space						
Exponent	1s	2s	3s	4s	5s	
	-873.663020	-128.327870	-24.571804	-3.927343	-0.253541	
69441980.	0.000001	0.000000	0.000000	0.000000	0.000000	
10392760.	0.000009	-0.000003	0.000001	-0.000001	0.000000	
2364302.	0.000046	-0.000015	0.000006	-0.000003	0.000001	
669532.6	0.000195	-0.000063	0.000027	-0.000011	0.000003	
218398.0	0.000713	-0.000229	0.000099	-0.000041	0.000010	
78839.46	0.002327	-0.000750	0.000324	-0.000134	0.000033	
30750.15	0.006946	-0.002252	0.000973	-0.000403	0.000099	
12756.26	0.019113	-0.006257	0.002705	-0.001123	0.000277	
5566.410	0.048244	-0.016210	0.007040	-0.002921	0.000716	
2534.179	0.109310	-0.038583	0.016849	-0.007013	0.001731	
1195.970	0.210942	-0.082682	0.036703	-0.015285	0.003740	
582.2144	0.313235	-0.148668	0.067750	-0.028459	0.007056	
291.0348	0.294795	-0.194893	0.093950	-0.039676	0.009666	
148.2206	0.128244	-0.080980	0.041799	-0.018353	0.004798	
72.81785	0.014043	0.315674	-0.204477	0.092786	-0.023703	
37.82028	-0.000135	0.563292	-0.520041	0.248781	-0.061344	
19.67215	0.000121	0.279878	-0.278405	0.147844	-0.040281	
9.453894	-0.000109	0.030055	0.579315	-0.392154	0.109841	
4.923336	0.000016	-0.000810	0.678868	-0.760265	0.211939	
2.347682	-0.000008	0.000475	0.117981	0.130242	-0.042832	
1.179603	0.000007	-0.000335	-0.001617	0.853165	-0.351536	
0.545542	-0.000001	0.000043	0.002069	0.390262	-0.244816	
0.110960	0.000000	-0.000012	-0.000160	0.009064	0.626981	
0.040291	0.000000	0.000004	0.000064	-0.002191	0.548868	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-118.889680	-20.734623	-2.642728		-13.720646	-0.657224
60999.06	0.000040	-0.000018	0.000007	1976.834	0.000218	-0.000071
14437.94	0.000353	-0.000158	0.000062	597.6371	0.002117	-0.000689
4689.369	0.002048	-0.000918	0.000360	233.1951	0.012196	-0.004002
1794.979	0.009112	-0.004117	0.001617	103.4678	0.047727	-0.015745
762.7074	0.032780	-0.015043	0.005914	49.35266	0.134455	-0.045143
348.7202	0.095459	-0.045225	0.017911	24.65115	0.266239	-0.089070
168.1859	0.214845	-0.106835	0.042608	12.53823	0.359690	-0.115122
84.18869	0.343002	-0.182139	0.073870	6.448772	0.295540	-0.063190
43.30313	0.325297	-0.163545	0.064744	3.280153	0.111362	0.138946
22.44578	0.140161	0.097809	-0.058701	1.613524	0.013554	0.355004
11.50290	0.018088	0.458968	-0.257028	0.758222	0.001028	0.399841
5.968877	0.001013	0.451965	-0.290278	0.338164	0.000213	0.261959
3.022031	-0.000125	0.126205	0.147575	0.137959	0.000089	0.075026
1.502096	0.000017	0.005941	0.560055			
0.708768	-0.000051	0.001397	0.420916			
0.299786	0.000004	-0.000096	0.077541			

Table XXXIV. Pd 3F ($26s16p13d$) basis set. Energy(E_H) = -4937.782764

Exponent	s space					
	1s	2s	3s	4s	5s	
	-873.663100	-128.327950	-24.571880	-3.927415	-0.253613	
106776400.	0.000001	0.000000	0.000000	0.000000	0.000000	
16026280.	0.000005	-0.000002	0.000001	0.000000	0.000000	
3655781.	0.000027	-0.000009	0.000004	-0.000002	0.000000	
1037722.	0.000113	-0.000036	0.000016	-0.000006	0.000002	
339236.2	0.000411	-0.000132	0.000057	-0.000024	0.000006	
122712.4	0.001339	-0.000431	0.000186	-0.000077	0.000019	
47956.81	0.004002	-0.001293	0.000558	-0.000232	0.000057	
19933.04	0.011081	-0.003606	0.001558	-0.000646	0.000159	
8715.081	0.028468	-0.009407	0.004073	-0.001692	0.000416	
3975.420	0.067096	-0.022922	0.009974	-0.004138	0.001016	
1879.753	0.140713	-0.051333	0.022531	-0.009391	0.002313	
916.4174	0.246572	-0.102280	0.045749	-0.019069	0.004684	
458.4438	0.319946	-0.167549	0.077572	-0.032716	0.008082	
233.7262	0.247015	-0.181579	0.089432	-0.037839	0.009289	
119.6972	0.076864	0.002389	-0.002061	0.000296	0.000049	
62.64175	0.003689	0.402203	-0.279526	0.128966	-0.032475	
33.21946	0.001156	0.524196	-0.518933	0.250565	-0.062662	
17.60455	-0.000585	0.209719	-0.167769	0.094046	-0.025406	
8.907469	0.000273	0.018265	0.631128	-0.445668	0.122318	
4.719738	-0.000201	0.000768	0.620771	-0.718555	0.206184	
2.317846	0.000105	-0.000198	0.104992	0.167208	-0.065561	
1.169549	-0.000048	-0.000049	-0.000275	0.835310	-0.326919	
0.551412	0.000017	-0.000037	0.001914	0.387206	-0.268058	
0.145656	-0.000006	0.000005	-0.000264	0.014517	0.325141	
0.067201	0.000004	-0.000004	0.000185	-0.004924	0.613395	
0.029733	-0.000001	0.000001	-0.000055	0.001180	0.251896	
	p space			d space		
Exponent	2p	3p	4p	Exponent	3d	4d
	-118.889750	-20.734696	-2.642797		-13.720719	-0.657295
60945.43	0.000040	-0.000018	0.000007	1974.971	0.000219	-0.000071
14426.45	0.000354	-0.000158	0.000062	597.0892	0.002121	-0.000691
4685.952	0.002051	-0.000919	0.000360	232.9947	0.012216	-0.004008
1793.772	0.009122	-0.004122	0.001618	103.3848	0.047787	-0.015765
762.2309	0.032810	-0.015057	0.005920	49.31574	0.134578	-0.045185
348.5167	0.095530	-0.045260	0.017925	24.63374	0.266368	-0.089110
168.0937	0.214952	-0.106893	0.042631	12.52993	0.359698	-0.115117
84.14585	0.343054	-0.182176	0.073886	6.444892	0.295369	-0.063068
43.28296	0.325189	-0.163444	0.064697	3.278323	0.111219	0.139128
22.43610	0.140028	0.098036	-0.058809	1.612745	0.013526	0.355041
11.49888	0.018056	0.459049	-0.257094	0.757956	0.001027	0.399705
5.967303	0.001013	0.451796	-0.290160	0.338099	0.000213	0.261890
3.021461	-0.000126	0.126119	0.147721	0.137934	0.000089	0.074998
1.501876	0.000017	0.005938	0.560048			
0.708719	-0.000052	0.001395	0.420802			
0.299831	0.000004	-0.000096	0.077560			

Table XXXV. Ag 2D ($22s14p11d$) basis set. Energy(E_H) = -5197.515700

Exponent	s space					
	1s	2s	3s	4s	5s	
	-914.032550	-135.083940	-26.122877	-4.188355	-0.259363	
26002930.	0.000004	-0.000001	0.000001	0.000000	0.000000	
3893496.	0.000032	-0.000010	0.000004	-0.000002	0.000000	
886054.9	0.000166	-0.000054	0.000023	-0.000010	0.000002	
250977.2	0.000702	-0.000226	0.000098	-0.000041	0.000010	
81881.09	0.002552	-0.000825	0.000358	-0.000150	0.000036	
29560.77	0.008271	-0.002684	0.001164	-0.000488	0.000118	
11529.51	0.024219	-0.007976	0.003473	-0.001456	0.000352	
4781.857	0.063784	-0.021633	0.009437	-0.003955	0.000958	
2085.223	0.146255	-0.053134	0.023467	-0.009869	0.002382	
947.7086	0.271435	-0.112856	0.050646	-0.021340	0.005181	
445.4889	0.349626	-0.190380	0.089422	-0.038081	0.009192	
213.6862	0.236245	-0.179319	0.089530	-0.038500	0.009445	
97.55628	0.046652	0.138884	-0.081852	0.036150	-0.009076	
49.80986	-0.003257	0.563379	-0.461523	0.220191	-0.053781	
25.06188	0.002008	0.422064	-0.458330	0.233948	-0.059695	
11.30207	-0.001159	0.065164	0.404870	-0.253207	0.068376	
5.898565	0.000711	-0.006313	0.781689	-0.818529	0.226270	
2.870115	-0.000375	0.002892	0.183663	-0.058821	0.012920	
1.387039	0.000169	-0.001265	0.002145	0.884450	-0.341130	
0.618410	-0.000047	0.000283	0.002104	0.463292	-0.275853	
0.116124	0.000009	-0.000057	-0.000134	0.011062	0.619590	
0.041902	-0.000004	0.000023	0.000057	-0.002887	0.550616	
	p space			d space		
Exponent	2p	3p	4p	Exponent	3d	4d
	-125.385430	-22.149014	-2.847218		-14.879905	-0.705602
30875.26	0.000141	-0.000063	0.000025	1077.717	0.000922	-0.000306
7312.175	0.001243	-0.000560	0.000221	324.8328	0.008425	-0.002841
2374.139	0.007036	-0.003194	0.001272	125.9607	0.042798	-0.014426
906.9794	0.029772	-0.013704	0.005437	54.86532	0.140214	-0.048455
383.9592	0.097039	-0.046189	0.018570	25.53386	0.298898	-0.102185
174.4242	0.233778	-0.117109	0.047144	12.18655	0.398999	-0.130900
83.05950	0.375661	-0.202401	0.083784	5.889268	0.279612	-0.026177
40.81030	0.324344	-0.149163	0.056654	2.733241	0.068788	0.263040
20.01061	0.105893	0.206259	-0.112524	1.221291	0.002624	0.448758
9.884051	0.005887	0.550604	-0.337946	0.511466	0.001182	0.368280
4.940968	0.001304	0.349468	-0.171080	0.192977	0.000030	0.133601
2.259630	-0.000529	0.046618	0.460779			
1.016750	0.000146	-0.000202	0.586776			
0.417689	-0.000057	0.000574	0.165152			

Table XXXVI. Ag 2D ($22s14p12d$) basis set. Energy(E_H) = -5197.516426

Exponent	s space				
	1s	2s	3s	4s	5s
	-914.032740	-135.084160	-26.123114	-4.188570	-0.259451
26016300.	0.000004	-0.000001	0.000001	0.000000	0.000000
3895476.	0.000032	-0.000010	0.000004	-0.000002	0.000000
886496.9	0.000166	-0.000054	0.000023	-0.000010	0.000002
251101.0	0.000702	-0.000226	0.000098	-0.000041	0.000010
81921.41	0.002551	-0.000824	0.000358	-0.000150	0.000036
29575.42	0.008266	-0.002683	0.001164	-0.000487	0.000118
11535.28	0.024204	-0.007971	0.003471	-0.001455	0.000351
4784.277	0.063747	-0.021620	0.009432	-0.003953	0.000958
2086.289	0.146181	-0.053104	0.023453	-0.009863	0.002381
948.1964	0.271341	-0.112804	0.050622	-0.021330	0.005179
445.7187	0.349621	-0.190328	0.089394	-0.038070	0.009191
213.7977	0.236386	-0.179418	0.089576	-0.038517	0.009450
97.62578	0.046737	0.138410	-0.081555	0.036009	-0.009041
49.84508	-0.003251	0.563180	-0.461165	0.220022	-0.053751
25.07914	0.002008	0.422501	-0.458847	0.234156	-0.059745
11.31177	-0.001160	0.065349	0.403540	-0.252141	0.068079
5.904747	0.000712	-0.006324	0.782048	-0.818453	0.226302
2.875007	-0.000375	0.002898	0.184433	-0.060739	0.013466
1.388300	0.000169	-0.001264	0.002243	0.884530	-0.341053
0.618791	-0.000047	0.000283	0.002096	0.464053	-0.276296
0.116189	0.000009	-0.000057	-0.000132	0.011084	0.619281
0.041925	-0.000004	0.000023	0.000056	-0.002888	0.550962

p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-125.385640	-22.149249	-2.847420		-14.880183	-0.705793
30833.54	0.000141	-0.000063	0.000025	1500.512	0.000449	-0.000150
7302.327	0.001246	-0.000561	0.000222	452.9389	0.004246	-0.001421
2370.946	0.007052	-0.003201	0.001275	176.3987	0.023172	-0.007827
905.7602	0.029835	-0.013733	0.005449	77.65016	0.083743	-0.028534
383.4411	0.097221	-0.046280	0.018606	36.69544	0.209098	-0.072502
174.1845	0.234109	-0.117287	0.047216	17.99281	0.346527	-0.116542
82.94279	0.375863	-0.202540	0.083846	8.969764	0.360233	-0.107019
40.75098	0.324009	-0.148749	0.056453	4.486903	0.181410	0.061372
19.97766	0.105502	0.207310	-0.113058	2.163768	0.031326	0.325819
9.867951	0.005815	0.550857	-0.338268	0.991712	0.001619	0.429243
4.933135	0.001307	0.348478	-0.169951	0.428961	0.000585	0.308824
2.256352	-0.000530	0.046330	0.461757	0.168533	0.000118	0.098273
1.015309	0.000146	-0.000192	0.586130			
0.417150	-0.000058	0.000570	0.164562			

Table XXXVII. Ag 2D ($22s14p13d$) basis set. Energy(E_H) = -5197.516666

Exponent	s space				
	1s	2s	3s	4s	5s
	-914.032810	-135.084240	-26.123204	-4.188652	-0.259486
26010390.	0.000004	-0.000001	0.000001	0.000000	0.000000
3894558.	0.000032	-0.000010	0.000004	-0.000002	0.000000
886283.6	0.000166	-0.000054	0.000023	-0.000010	0.000002
251039.7	0.000702	-0.000226	0.000098	-0.000041	0.000010
81901.25	0.002552	-0.000824	0.000358	-0.000150	0.000036
29568.07	0.008269	-0.002684	0.001164	-0.000487	0.000118
11532.39	0.024212	-0.007974	0.003472	-0.001456	0.000352
4783.063	0.063765	-0.021627	0.009434	-0.003954	0.000958
2085.753	0.146219	-0.053119	0.023460	-0.009866	0.002382
947.9508	0.271389	-0.112831	0.050634	-0.021335	0.005180
445.6030	0.349623	-0.190353	0.089408	-0.038076	0.009193
213.7424	0.236313	-0.179369	0.089554	-0.038508	0.009448
97.59435	0.046695	0.138631	-0.081694	0.036075	-0.009058
49.82870	-0.003252	0.563275	-0.461333	0.220104	-0.053773
25.07103	0.002007	0.422299	-0.458606	0.234059	-0.059727
11.30711	-0.001159	0.065261	0.404181	-0.252652	0.068226
5.901702	0.000711	-0.006318	0.781899	-0.818525	0.226332
2.872392	-0.000375	0.002895	0.184048	-0.059751	0.013172
1.387612	0.000169	-0.001265	0.002183	0.884534	-0.341139
0.618581	-0.000047	0.000283	0.002103	0.463611	-0.276124
0.116213	0.000009	-0.000057	-0.000133	0.011067	0.619241
0.041929	-0.000004	0.000023	0.000057	-0.002880	0.551047

Exponent	p space			Exponent	d space	
	2p	3p	4p		3d	4d
	-125.385720	-22.149338	-2.847497		-14.880286	-0.705865
30838.74	0.000141	-0.000063	0.000025	2083.467	0.000218	-0.000073
7303.553	0.001246	-0.000561	0.000222	629.9597	0.002119	-0.000708
2371.342	0.007050	-0.003200	0.001275	245.8548	0.012223	-0.004118
905.9123	0.029827	-0.013729	0.005448	109.1257	0.047950	-0.016237
383.5080	0.097197	-0.046268	0.018602	52.08560	0.135310	-0.046680
174.2165	0.234064	-0.117263	0.047206	26.03758	0.268099	-0.092096
82.95849	0.375836	-0.202521	0.083838	13.26124	0.361381	-0.118870
40.75892	0.324055	-0.148804	0.056480	6.837103	0.293058	-0.061330
19.98202	0.105554	0.207170	-0.112988	3.485695	0.107687	0.149609
9.870116	0.005824	0.550819	-0.338221	1.722271	0.012822	0.360773
4.934235	0.001307	0.348609	-0.170114	0.812640	0.001226	0.394770
2.256887	-0.000530	0.046372	0.461596	0.363334	0.000320	0.253809
1.015553	0.000146	-0.000193	0.586240	0.148420	0.000124	0.071333
0.417240	-0.000058	0.000570	0.164655			

Table XXXVIII. Ag 2D ($23s15p12d$) basis set. Energy(E_H) = -5197.516966

Exponent	s space				
	1s	2s	3s	4s	5s
	-914.032850	-135.084290	-26.123241	-4.188679	-0.259559
26822000.	0.000004	-0.000001	0.000001	0.000000	0.000000
4015047.	0.000030	-0.000010	0.000004	-0.000002	0.000000
913504.5	0.000160	-0.000052	0.000022	-0.000009	0.000002
258701.0	0.000676	-0.000218	0.000094	-0.000040	0.000010
84385.86	0.002459	-0.000794	0.000345	-0.000144	0.000035
30459.99	0.007973	-0.002587	0.001122	-0.000470	0.000114
11878.36	0.023371	-0.007691	0.003348	-0.001404	0.000340
4925.785	0.061685	-0.020894	0.009115	-0.003819	0.000924
2147.641	0.142106	-0.051435	0.022700	-0.009550	0.002313
975.8607	0.266199	-0.109942	0.049301	-0.020757	0.005023
458.5688	0.349360	-0.187550	0.087869	-0.037436	0.009092
219.9530	0.244095	-0.184506	0.091901	-0.039413	0.009553
101.3055	0.051521	0.114078	-0.066472	0.028983	-0.007008
51.71795	-0.002983	0.551494	-0.441899	0.210575	-0.052147
26.00893	0.002073	0.444900	-0.483913	0.244657	-0.060905
11.83801	-0.001230	0.075945	0.332788	-0.198985	0.050475
6.238837	0.000780	-0.007085	0.797533	-0.804331	0.228290
3.121696	-0.000418	0.003445	0.227441	-0.168776	0.035824
1.479743	0.000189	-0.001462	0.007119	0.859157	-0.308422
0.662015	-0.000063	0.000395	0.001966	0.526825	-0.321202
0.158303	0.000025	-0.000164	-0.000194	0.025211	0.245622
0.078664	-0.000019	0.000120	0.000158	-0.010494	0.605490
0.033620	0.000005	-0.000033	-0.000044	0.002299	0.324888

p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-125.385800	-22.149385	-2.847547		-14.880307	-0.705899
44192.19	0.000075	-0.000034	0.000013	1499.060	0.000449	-0.000150
10462.63	0.000668	-0.000301	0.000120	452.5038	0.004255	-0.001424
3397.791	0.003837	-0.001735	0.000688	176.2303	0.023213	-0.007841
1299.594	0.016704	-0.007641	0.003043	77.57503	0.083869	-0.028577
551.3113	0.057662	-0.026959	0.010749	36.65788	0.209354	-0.072592
251.4835	0.154804	-0.075587	0.030467	17.97144	0.346809	-0.116625
120.6669	0.301840	-0.156294	0.063509	8.957425	0.360145	-0.106913
60.04244	0.372071	-0.203025	0.083977	4.479784	0.180976	0.061977
30.47058	0.225841	-0.032863	0.002349	2.159863	0.031143	0.326318
15.23179	0.046667	0.364464	-0.199489	0.990078	0.001611	0.428924
7.735713	0.001192	0.529627	-0.342938	0.428481	0.000583	0.308337
3.923810	0.000550	0.212028	-0.002207	0.168386	0.000118	0.098128
1.906791	-0.000265	0.017806	0.534853			
0.878535	0.000038	0.001376	0.504879			
0.367924	-0.000023	0.000041	0.114755			

Table XXXIX. Ag 2D ($23s15p12d$) basis set. Energy(E_H) = -5197.517028

Exponent	s space				
	1s	2s	3s	4s	5s
	-914.032830	-135.084220	-26.123175	-4.188619	-0.259482
44841640.	0.000002	-0.000001	0.000000	0.000000	0.000000
6713677.	0.000016	-0.000005	0.000002	-0.000001	0.000000
1527831.	0.000084	-0.000027	0.000012	-0.000005	0.000001
432772.2	0.000356	-0.000115	0.000050	-0.000021	0.000005
141198.6	0.001295	-0.000418	0.000181	-0.000076	0.000018
50979.93	0.004218	-0.001365	0.000593	-0.000248	0.000060
19886.43	0.012507	-0.004075	0.001769	-0.000741	0.000180
8250.221	0.033877	-0.011259	0.004908	-0.002057	0.000496
3600.107	0.082730	-0.028532	0.012478	-0.005237	0.001271
1638.701	0.174664	-0.065539	0.029072	-0.012224	0.002948
773.0857	0.293057	-0.128675	0.058228	-0.024609	0.005989
375.8499	0.329871	-0.195509	0.093057	-0.039651	0.009548
186.1225	0.187108	-0.141819	0.072020	-0.031271	0.007760
87.00573	0.029488	0.221200	-0.136580	0.061654	-0.015479
44.81045	-0.002001	0.572515	-0.497150	0.238613	-0.058132
22.95594	0.001152	0.355216	-0.381780	0.199342	-0.051786
10.64854	-0.000667	0.046766	0.497128	-0.327416	0.089483
5.547514	0.000367	-0.003319	0.737144	-0.803242	0.221502
2.664866	-0.000194	0.001559	0.147570	0.044872	-0.017632
1.320447	0.000093	-0.000780	-0.000493	0.873324	-0.344997
0.599363	-0.000026	0.000157	0.002201	0.423437	-0.256785
0.116337	0.000005	-0.000032	-0.000161	0.009824	0.620575
0.041910	-0.000002	0.000013	0.000066	-0.002472	0.550861

p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-125.385730	-22.149317	-2.847485		-14.880240	-0.705833
44185.48	0.000075	-0.000034	0.000013	1498.908	0.000450	-0.000150
10461.18	0.000668	-0.000301	0.000120	452.4602	0.004255	-0.001424
3397.386	0.003838	-0.001735	0.000688	176.2126	0.023217	-0.007842
1299.466	0.016706	-0.007642	0.003043	77.56600	0.083887	-0.028584
551.2659	0.057668	-0.026962	0.010750	36.65285	0.209390	-0.072604
251.4635	0.154820	-0.075595	0.030470	17.96881	0.346830	-0.116633
120.6565	0.301861	-0.156306	0.063514	8.956243	0.360116	-0.106896
60.03720	0.372065	-0.203021	0.083975	4.479294	0.180934	0.062009
30.46826	0.225810	-0.032828	0.002333	2.159762	0.031133	0.326313
15.23136	0.046656	0.364452	-0.199485	0.990034	0.001612	0.428946
7.735924	0.001193	0.529588	-0.342903	0.428467	0.000582	0.308293
3.924171	0.000550	0.212049	-0.002317	0.168399	0.000118	0.098128
1.907330	-0.000265	0.017819	0.534643			
0.878841	0.000038	0.001378	0.505067			
0.368031	-0.000023	0.000041	0.114852			

Table XL. Ag 2D (23s15p13d) basis set. Energy(E_H) = -5197.517206

Exponent	s space				
	1s	2s	3s	4s	5s
	-914.032920	-135.084370	-26.123330	-4.188761	-0.259593
26698700.	0.000004	-0.000001	0.000001	0.000000	0.000000
3998300.	0.000031	-0.000010	0.000004	-0.000002	0.000000
910057.5	0.000161	-0.000052	0.000022	-0.000009	0.000002
257815.7	0.000679	-0.000219	0.000095	-0.000040	0.000010
84123.07	0.002468	-0.000797	0.000346	-0.000145	0.000035
30373.49	0.007999	-0.002596	0.001126	-0.000471	0.000114
11847.56	0.023438	-0.007713	0.003358	-0.001408	0.000341
4914.106	0.061836	-0.020948	0.009138	-0.003829	0.000926
2142.981	0.142377	-0.051547	0.022750	-0.009571	0.002319
973.9248	0.266499	-0.110116	0.049383	-0.020792	0.005032
457.7394	0.349318	-0.187691	0.087946	-0.037468	0.009100
219.5871	0.243600	-0.184191	0.091763	-0.039359	0.009541
101.1073	0.051247	0.115318	-0.067249	0.029343	-0.007098
51.62389	-0.002999	0.552023	-0.442750	0.210993	-0.052252
25.96611	0.002072	0.443760	-0.482819	0.244203	-0.060803
11.82216	-0.001228	0.075461	0.335177	-0.200766	0.050964
6.227645	0.000778	-0.006999	0.797322	-0.804910	0.228475
3.112378	-0.000418	0.003408	0.225932	-0.165928	0.034938
1.478182	0.000190	-0.001454	0.006834	0.859327	-0.308497
0.661667	-0.000063	0.000392	0.002013	0.525865	-0.320951
0.158775	0.000025	-0.000163	-0.000210	0.025189	0.243531
0.078877	-0.000019	0.000119	0.000169	-0.010427	0.606403
0.033664	0.000005	-0.000033	-0.000047	0.002279	0.326172

Exponent	p space			Exponent	d space	
	2p	3p	4p		3d	4d
	-125.385880	-22.149473	-2.847624		-14.880410	-0.705971
44130.38	0.000075	-0.000034	0.000013	2085.663	0.000218	-0.000073
10448.39	0.000670	-0.000302	0.000120	630.6593	0.002114	-0.000706
3393.286	0.003846	-0.001739	0.000689	246.1405	0.012195	-0.004108
1297.908	0.016739	-0.007657	0.003049	109.2597	0.047847	-0.016202
550.6051	0.057770	-0.027012	0.010770	52.15428	0.135052	-0.046589
251.1610	0.155046	-0.075711	0.030517	26.07662	0.267701	-0.091966
120.5097	0.302137	-0.156468	0.063583	13.28417	0.361182	-0.118820
59.96284	0.372040	-0.202994	0.083959	6.849834	0.293480	-0.061720
30.42866	0.225417	-0.032213	0.002042	3.492494	0.108158	0.148964
15.20941	0.046444	0.365344	-0.200017	1.724817	0.012922	0.360884
7.723918	0.001181	0.529407	-0.342863	0.813283	0.001223	0.395121
3.917010	0.000546	0.211216	-0.000915	0.363560	0.000322	0.253930
1.904064	-0.000263	0.017642	0.535294	0.148508	0.000124	0.071485
0.877441	0.000037	0.001385	0.504158			
0.367504	-0.000023	0.000038	0.114368			

Table XLI. Ag 2D (23s16p13d) basis set. Energy(E_H) = -5197.517396

Exponent	s space				
	1s	2s	3s	4s	5s
	-914.032940	-135.084390	-26.123355	-4.188778	-0.259607
26708950.	0.000004	-0.000001	0.000001	0.000000	0.000000
3999084.	0.000031	-0.000010	0.000004	-0.000002	0.000000
910062.7	0.000161	-0.000052	0.000022	-0.000009	0.000002
257774.1	0.000679	-0.000219	0.000095	-0.000040	0.000010
84098.24	0.002469	-0.000797	0.000346	-0.000145	0.000035
30361.22	0.008003	-0.002597	0.001127	-0.000472	0.000114
11841.68	0.023455	-0.007719	0.003360	-0.001409	0.000341
4911.259	0.061883	-0.020964	0.009145	-0.003832	0.000927
2141.577	0.142482	-0.051590	0.022770	-0.009579	0.002321
973.2217	0.266652	-0.110196	0.049419	-0.020809	0.005036
457.3822	0.349360	-0.187787	0.087999	-0.037489	0.009105
219.3997	0.243401	-0.184060	0.091701	-0.039338	0.009538
100.9772	0.051094	0.116119	-0.067734	0.029575	-0.007159
51.55907	-0.003018	0.552461	-0.443447	0.211321	-0.052327
25.93306	0.002073	0.443034	-0.481979	0.243884	-0.060746
11.79973	-0.001228	0.075075	0.337935	-0.202876	0.051571
6.213818	0.000778	-0.007008	0.796968	-0.805555	0.228626
3.101426	-0.000418	0.003408	0.224081	-0.162330	0.033912
1.475901	0.000191	-0.001461	0.006532	0.859869	-0.308895
0.660832	-0.000064	0.000394	0.002054	0.524392	-0.320344
0.158485	0.000025	-0.000163	-0.000224	0.024980	0.245754
0.078648	-0.000019	0.000119	0.000179	-0.010325	0.605830
0.033614	0.000005	-0.000033	-0.000050	0.002264	0.324647

p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-125.385920	-22.149504	-2.847647		-14.880433	-0.705986
64635.06	0.000039	-0.000017	0.000007	2084.389	0.000218	-0.000073
15298.61	0.000345	-0.000155	0.000062	630.2375	0.002117	-0.000707
4968.942	0.002003	-0.000904	0.000358	245.9626	0.012213	-0.004114
1902.047	0.008921	-0.004057	0.001613	109.1741	0.047914	-0.016224
808.2751	0.032146	-0.014847	0.005910	52.11019	0.135217	-0.046646
369.6123	0.093880	-0.044753	0.017947	26.05171	0.267956	-0.092051
178.3190	0.212268	-0.106221	0.042900	13.26908	0.361352	-0.118859
89.31273	0.341224	-0.182342	0.074911	6.840702	0.293239	-0.061470
45.97953	0.327263	-0.166686	0.066949	3.486941	0.107818	0.149612
23.87284	0.143668	0.092096	-0.056978	1.721593	0.012831	0.361252
12.25848	0.019093	0.457602	-0.261075	0.811806	0.001220	0.394763
6.381264	0.000978	0.455126	-0.296401	0.363068	0.000320	0.253399
3.242583	-0.000115	0.128313	0.150353	0.148369	0.000124	0.071330
1.613768	0.000000	0.006392	0.562531			
0.761948	-0.000050	0.001426	0.418999			
0.322818	0.000003	-0.000075	0.076980			

Table XLII. Ag 2D ($24s16p13d$) basis set. Energy(E_H) = -5197.517526

s space					
Exponent	1s	2s	3s	4s	5s
	-914.033000	-135.084410	-26.123369	-4.188792	-0.259610
45799420.	0.000002	-0.000001	0.000000	0.000000	0.000000
6856793.	0.000016	-0.000005	0.000002	-0.000001	0.000000
1560327.	0.000082	-0.000026	0.000011	-0.000005	0.000001
441958.0	0.000346	-0.000112	0.000048	-0.000020	0.000005
144190.9	0.001262	-0.000407	0.000176	-0.000074	0.000018
52059.14	0.004110	-0.001330	0.000578	-0.000242	0.000059
20307.08	0.012191	-0.003971	0.001724	-0.000722	0.000175
8424.626	0.033051	-0.010976	0.004784	-0.002005	0.000485
3676.139	0.080861	-0.027850	0.012178	-0.005110	0.001237
1673.223	0.171394	-0.064109	0.028423	-0.011953	0.002893
789.2500	0.289853	-0.126519	0.057206	-0.024165	0.005858
383.5573	0.331341	-0.194280	0.092298	-0.039335	0.009538
189.7782	0.192992	-0.147152	0.074594	-0.032316	0.007877
88.84655	0.031813	0.205294	-0.125827	0.056581	-0.013891
45.83910	-0.002114	0.568589	-0.487112	0.233550	-0.057671
23.48886	0.001260	0.369665	-0.401042	0.207939	-0.052425
10.91931	-0.000739	0.051845	0.458841	-0.296189	0.077714
5.721080	0.000423	-0.003850	0.752266	-0.803064	0.227531
2.793857	-0.000232	0.001908	0.167994	-0.025775	-0.006667
1.383787	0.000115	-0.000948	0.000858	0.864309	-0.318078
0.630497	-0.000037	0.000231	0.002482	0.467018	-0.296994
0.153527	0.000014	-0.000091	-0.000373	0.019514	0.296157
0.073135	-0.000010	0.000065	0.000276	-0.007701	0.602850
0.031995	0.000003	-0.000019	-0.000082	0.001822	0.281869

p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-125.385930	-22.149514	-2.847657		-14.880443	-0.705995
64614.40	0.000039	-0.000017	0.000007	2084.053	0.000218	-0.000073
15293.49	0.000346	-0.000156	0.000062	630.1613	0.002117	-0.000707
4967.243	0.002004	-0.000905	0.000359	245.9387	0.012215	-0.004115
1901.392	0.008926	-0.004059	0.001614	109.1650	0.047919	-0.016226
807.9971	0.032163	-0.014855	0.005913	52.10669	0.135225	-0.046649
369.4871	0.093923	-0.044774	0.017956	26.05023	0.267967	-0.092055
178.2599	0.212338	-0.106259	0.042915	13.26824	0.361362	-0.118862
89.28259	0.341283	-0.182379	0.074928	6.840174	0.293226	-0.061457
45.96275	0.327216	-0.166630	0.066921	3.486618	0.107798	0.149651
23.86289	0.143559	0.092340	-0.057098	1.721429	0.012825	0.361257
12.25264	0.019055	0.457832	-0.261237	0.811754	0.001221	0.394744
6.377970	0.000978	0.454937	-0.296249	0.363044	0.000320	0.253388
3.240587	-0.000116	0.128106	0.150847	0.148357	0.000124	0.071315
1.612861	0.000001	0.006364	0.562524			
0.761647	-0.000050	0.001427	0.418694			
0.322736	0.000003	-0.000075	0.076910			

Table XLIII. Ag 2D ($24s16p13d$) basis set. Energy(E_H) = -5197.517520

s space						
Exponent	1s	2s	3s	4s	5s	
	-914.032950	-135.084340	-26.123299	-4.188724	-0.259532	
73304660.	0.000001	0.000000	0.000000	0.000000	0.000000	
10972750.	0.000009	-0.000003	0.000001	-0.000001	0.000000	
2496487.	0.000046	-0.000015	0.000006	-0.000003	0.000001	
706982.8	0.000193	-0.000062	0.000027	-0.000011	0.000003	
230620.2	0.000703	-0.000227	0.000098	-0.000041	0.000010	
83254.57	0.002295	-0.000741	0.000321	-0.000135	0.000033	
32473.80	0.006849	-0.002224	0.000966	-0.000404	0.000098	
13472.14	0.018850	-0.006180	0.002685	-0.001126	0.000273	
5879.241	0.047607	-0.016016	0.006992	-0.002929	0.000706	
2676.830	0.108006	-0.038149	0.016745	-0.007038	0.001710	
1263.426	0.208973	-0.081888	0.036535	-0.015363	0.003700	
615.1442	0.311925	-0.147724	0.067648	-0.028700	0.007004	
307.5739	0.296483	-0.195193	0.094546	-0.040319	0.009667	
156.6993	0.131371	-0.085086	0.044142	-0.019575	0.005026	
76.91626	0.014854	0.309337	-0.201211	0.092323	-0.023238	
39.98682	-0.000223	0.563956	-0.521843	0.252307	-0.061241	
20.82010	0.000168	0.285628	-0.288803	0.155717	-0.041754	
10.01903	-0.000134	0.031320	0.577332	-0.398441	0.110214	
5.239965	0.000031	-0.000984	0.682885	-0.772843	0.212076	
2.514706	-0.000016	0.000517	0.120355	0.139358	-0.045643	
1.258485	0.000011	-0.000354	-0.001047	0.856289	-0.347198	
0.581157	-0.000002	0.000047	0.002020	0.386144	-0.237892	
0.116398	0.000000	-0.000012	-0.000147	0.008745	0.621963	
0.041882	0.000000	0.000005	0.000059	-0.002130	0.550379	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-125.385860	-22.149442	-2.847589		-14.880372	-0.705925
64583.09	0.000039	-0.000017	0.000007	2083.282	0.000218	-0.000073
15286.46	0.000346	-0.000156	0.000062	629.9434	0.002119	-0.000708
4965.095	0.002006	-0.000905	0.000359	245.8583	0.012222	-0.004118
1900.608	0.008932	-0.004062	0.001615	109.1307	0.047944	-0.016235
807.6726	0.032183	-0.014865	0.005917	52.09082	0.135279	-0.046668
369.3408	0.093973	-0.044799	0.017966	26.04209	0.268039	-0.092079
178.1877	0.212431	-0.106309	0.042936	13.26376	0.361395	-0.118869
89.24407	0.341363	-0.182429	0.074950	6.837694	0.293148	-0.061384
45.94120	0.327152	-0.166554	0.066883	3.485203	0.107707	0.149804
23.85042	0.143418	0.092636	-0.057241	1.720725	0.012802	0.361311
12.24601	0.019009	0.458058	-0.261404	0.811419	0.001221	0.394726
6.374524	0.000978	0.454713	-0.296066	0.362879	0.000319	0.253254
3.238622	-0.000118	0.127897	0.151308	0.148309	0.000124	0.071245
1.612095	0.000001	0.006337	0.562463			
0.761398	-0.000051	0.001429	0.418488			
0.322610	0.000003	-0.000076	0.076824			

Table XLIV. Ag 2D (24s16p14d) basis set. Energy(E_H) = -5197.517603

s space						
Exponent	1s	2s	3s	4s	5s	
	-914.033030	-135.084440	-26.123400	-4.188821	-0.259622	
45775570.	0.000002	-0.000001	0.000000	0.000000	0.000000	
6853642.	0.000016	-0.000005	0.000002	-0.000001	0.000000	
1559695.	0.000082	-0.000026	0.000011	-0.000005	0.000001	
441801.2	0.000347	-0.000112	0.000048	-0.000020	0.000005	
144146.7	0.001262	-0.000407	0.000176	-0.000074	0.000018	
52045.42	0.004111	-0.001331	0.000578	-0.000242	0.000059	
20302.47	0.012194	-0.003972	0.001724	-0.000722	0.000175	
8422.973	0.033057	-0.010979	0.004785	-0.002006	0.000485	
3675.515	0.080873	-0.027855	0.012180	-0.005110	0.001237	
1672.980	0.171412	-0.064117	0.028427	-0.011955	0.002894	
789.1535	0.289864	-0.126528	0.057211	-0.024167	0.005858	
383.5187	0.331326	-0.194281	0.092299	-0.039335	0.009538	
189.7629	0.192964	-0.147127	0.074582	-0.032311	0.007876	
88.83981	0.031805	0.205349	-0.125864	0.056598	-0.013896	
45.83569	-0.002114	0.568598	-0.487141	0.233564	-0.057674	
23.48723	0.001260	0.369618	-0.400982	0.207914	-0.052422	
10.91855	-0.000738	0.051830	0.458942	-0.296276	0.077743	
5.720647	0.000423	-0.003849	0.752220	-0.803048	0.227522	
2.793581	-0.000232	0.001908	0.167946	-0.025659	-0.006688	
1.383724	0.000115	-0.000947	0.000854	0.864292	-0.318105	
0.630477	-0.000037	0.000231	0.002482	0.466989	-0.296955	
0.153447	0.000013	-0.000091	-0.000373	0.019515	0.296579	
0.073110	-0.000010	0.000065	0.000276	-0.007713	0.602488	
0.031994	0.000003	-0.000019	-0.000082	0.001827	0.281803	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-125.385960	-22.149545	-2.847684		-14.880479	-0.706020
64578.75	0.000039	-0.000017	0.000007	0.132865	0.000089	0.052519
15285.63	0.000346	-0.000156	0.000062	0.314253	0.000264	0.208513
4964.797	0.002006	-0.000905	0.000359	0.683094	0.000874	0.357348
1900.479	0.008933	-0.004063	0.001615	1.414352	0.005735	0.373098
807.6110	0.032187	-0.014867	0.005918	2.814937	0.061337	0.217641
369.3086	0.093985	-0.044805	0.017968	5.402076	0.217939	-0.002065
178.1724	0.212446	-0.106317	0.042939	10.17037	0.342747	-0.107229
89.23821	0.341361	-0.182429	0.074951	19.27920	0.307338	-0.103883
45.93930	0.327133	-0.166541	0.066876	37.01607	0.189241	-0.065604
23.84988	0.143409	0.092650	-0.057245	73.09129	0.082677	-0.028215
12.24560	0.019008	0.458087	-0.261429	151.7839	0.026767	-0.009051
6.374099	0.000977	0.454716	-0.296054	340.2119	0.006364	-0.002134
3.238192	-0.000117	0.127863	0.151414	870.4871	0.001060	-0.000355
1.611764	0.000001	0.006329	0.562581	2874.886	0.000107	-0.000036
0.761186	-0.000050	0.001428	0.418339			
0.322541	0.000003	-0.000076	0.076767			

Table XLV. Ag 2D ($24s17p14d$) basis set. Energy(E_H) = -5197.517676

s space						
Exponent	1s	2s	3s	4s	5s	
	-914.033030	-135.084450	-26.123410	-4.188828	-0.259628	
45781970.	0.000002	-0.000001	0.000000	0.000000	0.000000	
6854415.	0.000016	-0.000005	0.000002	-0.000001	0.000000	
1559811.	0.000082	-0.000026	0.000011	-0.000005	0.000001	
441820.1	0.000347	-0.000112	0.000048	-0.000020	0.000005	
144149.5	0.001262	-0.000407	0.000176	-0.000074	0.000018	
52045.53	0.004111	-0.001331	0.000578	-0.000242	0.000059	
20302.23	0.012194	-0.003972	0.001724	-0.000722	0.000175	
8422.756	0.033059	-0.010979	0.004785	-0.002006	0.000485	
3675.370	0.080878	-0.027856	0.012181	-0.005111	0.001237	
1672.890	0.171424	-0.064122	0.028429	-0.011955	0.002894	
789.0978	0.289883	-0.126539	0.057216	-0.024169	0.005859	
383.4840	0.331331	-0.194292	0.092306	-0.039338	0.009539	
189.7423	0.192936	-0.147105	0.074570	-0.032307	0.007876	
88.83018	0.031789	0.205443	-0.125924	0.056628	-0.013905	
45.82925	-0.002111	0.568638	-0.487222	0.233600	-0.057682	
23.48353	0.001258	0.369531	-0.400847	0.207862	-0.052414	
10.91567	-0.000737	0.051793	0.459326	-0.296601	0.077842	
5.718772	0.000422	-0.003851	0.752094	-0.803054	0.227514	
2.792070	-0.000231	0.001908	0.167717	-0.025000	-0.006872	
1.383202	0.000115	-0.000948	0.000827	0.864329	-0.318194	
0.630268	-0.000037	0.000231	0.002483	0.466646	-0.296796	
0.153380	0.000013	-0.000091	-0.000373	0.019455	0.297179	
0.073039	-0.000010	0.000065	0.000277	-0.007676	0.602538	
0.031970	0.000003	-0.000019	-0.000082	0.001820	0.281182	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-125.385980	-22.149558	-2.847693		-14.880489	-0.706027
94538.77	0.000020	-0.000009	0.000004	0.132812	0.000089	0.052472
22372.75	0.000178	-0.000080	0.000032	0.314074	0.000263	0.208300
7267.093	0.001040	-0.000469	0.000186	0.682579	0.000874	0.357203
2783.005	0.004710	-0.002133	0.000846	1.413415	0.005720	0.373259
1184.192	0.017503	-0.008017	0.003193	2.813822	0.061296	0.217856
542.6203	0.054181	-0.025358	0.010111	5.401216	0.217962	-0.002023
262.8041	0.136308	-0.066330	0.026724	10.17057	0.342831	-0.107255
132.5444	0.262617	-0.134844	0.054678	19.28188	0.307353	-0.103889
68.87181	0.349133	-0.190307	0.078740	37.02266	0.189208	-0.065592
36.47887	0.262614	-0.101552	0.036205	73.10434	0.082654	-0.028208
19.31598	0.085316	0.206433	-0.113556	151.8114	0.026759	-0.009048
10.20832	0.007468	0.494334	-0.296249	340.2782	0.006361	-0.002133
5.448732	0.000842	0.365045	-0.221345	870.6747	0.001060	-0.000355
2.812278	-0.000259	0.079918	0.262447	2875.574	0.000107	-0.000036
1.410943	0.000045	0.003338	0.561103			
0.676946	-0.000055	0.000974	0.349023			
0.287128	0.000006	-0.000039	0.053085			

Table XLVI. Ag 2D (25s17p13d) basis set. Energy(E_H) = -5197.517657

s space						
Exponent	1s	2s	3s	4s	5s	
	-914.033030	-135.084430	-26.123386	-4.188805	-0.259617	
76244910.	0.000001	0.000000	0.000000	0.000000	0.000000	
11408230.	0.000008	-0.000003	0.000001	0.000000	0.000000	
2595418.	0.000043	-0.000014	0.000006	-0.000003	0.000001	
734991.0	0.000184	-0.000059	0.000026	-0.000011	0.000003	
239741.6	0.000670	-0.000216	0.000094	-0.000039	0.000009	
86539.61	0.002187	-0.000706	0.000306	-0.000128	0.000031	
33751.81	0.006531	-0.002120	0.000921	-0.000385	0.000093	
14000.85	0.017995	-0.005895	0.002561	-0.001074	0.000260	
6109.319	0.045547	-0.015298	0.006677	-0.002798	0.000677	
2781.387	0.103779	-0.036529	0.016026	-0.006734	0.001631	
1312.776	0.202508	-0.078793	0.035120	-0.014770	0.003573	
639.2330	0.307375	-0.143581	0.065611	-0.027811	0.006751	
319.6938	0.301739	-0.194588	0.093907	-0.040052	0.009700	
162.8414	0.141980	-0.098210	0.050762	-0.022339	0.005493	
79.51284	0.017798	0.284751	-0.182674	0.083432	-0.020582	
41.39659	-0.000527	0.564532	-0.512041	0.247090	-0.060942	
21.55181	0.000351	0.307026	-0.321125	0.170787	-0.043606	
10.32427	-0.000234	0.036845	0.536443	-0.361696	0.096244	
5.422493	0.000092	-0.001617	0.706487	-0.782640	0.221600	
2.639894	-0.000050	0.000865	0.139352	0.063219	-0.033701	
1.322785	0.000028	-0.000514	-0.000346	0.856390	-0.320986	
0.611289	-0.000008	0.000101	0.002368	0.429530	-0.281304	
0.153218	0.000003	-0.000042	-0.000356	0.016819	0.309526	
0.071620	-0.000002	0.000029	0.000257	-0.006238	0.606039	
0.031442	0.000001	-0.000009	-0.000077	0.001496	0.268105	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-125.385950	-22.149531	-2.847669		-14.880457	-0.706005
94658.22	0.000020	-0.000009	0.000004	2082.525	0.000219	-0.000073
22401.41	0.000178	-0.000080	0.000032	629.6503	0.002121	-0.000709
7276.528	0.001038	-0.000468	0.000186	245.7252	0.012236	-0.004122
2786.677	0.004699	-0.002128	0.000844	109.0638	0.047998	-0.016253
1185.788	0.017465	-0.007999	0.003186	52.05505	0.135415	-0.046716
543.3686	0.054068	-0.025304	0.010089	26.02236	0.268219	-0.092136
263.1771	0.136061	-0.066204	0.026673	13.25319	0.361446	-0.118876
132.7417	0.262271	-0.134648	0.054598	6.832263	0.292947	-0.061216
68.97937	0.349034	-0.190241	0.078709	3.482386	0.107513	0.150083
36.53901	0.263014	-0.102085	0.036466	1.719484	0.012760	0.361348
19.35069	0.085697	0.205403	-0.113033	0.811032	0.001221	0.394490
10.22626	0.007542	0.494019	-0.295893	0.362824	0.000318	0.253156
5.458158	0.000842	0.365941	-0.222266	0.148283	0.000124	0.071240
2.817396	-0.000258	0.080395	0.261098			
1.413484	0.000044	0.003371	0.561176			
0.678095	-0.000055	0.000978	0.349961			
0.287657	0.000006	-0.000039	0.053396			

Table XLVII. Ag 2D (26s16p13d) basis set. Energy(E_H) = -5197.517613

Exponent	s space				
	1s	2s	3s	4s	5s
	-914.033040	-135.084420	-26.123383	-4.188804	-0.259611
112846900.	0.000001	0.000000	0.000000	0.000000	0.000000
16959820.	0.000005	-0.000002	0.000001	0.000000	0.000000
3877170.	0.000026	-0.000008	0.000004	-0.000002	0.000000
1102756.	0.000110	-0.000035	0.000015	-0.000006	0.000002
360988.9	0.000401	-0.000129	0.000056	-0.000023	0.000006
130655.5	0.001307	-0.000422	0.000183	-0.000077	0.000019
51045.50	0.003911	-0.001265	0.000549	-0.000230	0.000056
21197.48	0.010849	-0.003536	0.001536	-0.000643	0.000155
9258.205	0.027925	-0.009238	0.004020	-0.001687	0.000409
4219.809	0.065931	-0.022542	0.009859	-0.004130	0.000998
1994.505	0.138615	-0.050556	0.022301	-0.009387	0.002276
972.2558	0.243970	-0.101021	0.045411	-0.019113	0.004621
486.4668	0.319230	-0.166332	0.077348	-0.032944	0.008011
248.1980	0.250302	-0.183077	0.090574	-0.038699	0.009351
127.4637	0.080378	-0.005421	0.002169	-0.001567	0.000504
66.56795	0.004373	0.393868	-0.273870	0.127674	-0.031657
35.32009	0.001082	0.527748	-0.522445	0.254927	-0.062775
18.75558	-0.000544	0.217768	-0.182828	0.103714	-0.027499
9.468980	0.000250	0.019883	0.628833	-0.451912	0.122359
5.031817	-0.000189	0.000493	0.627061	-0.731620	0.206708
2.482671	0.000098	-0.000099	0.107595	0.175089	-0.067780
1.248204	-0.000044	-0.000099	0.000184	0.839149	-0.323176
0.587131	0.000016	-0.000022	0.001873	0.383211	-0.260758
0.152589	-0.000005	0.000000	-0.000241	0.013936	0.325674
0.069830	0.000003	0.000000	0.000170	-0.004793	0.609980
0.030737	-0.000001	0.000000	-0.000052	0.001163	0.251231

p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-125.385940	-22.149523	-2.847665		-14.880453	-0.706003
64373.72	0.000039	-0.000018	0.000007	2080.460	0.000219	-0.000073
15240.49	0.000348	-0.000156	0.000062	629.1563	0.002124	-0.000710
4951.311	0.002015	-0.000909	0.000360	245.5741	0.012249	-0.004127
1895.713	0.008968	-0.004079	0.001622	109.0126	0.048027	-0.016263
805.7325	0.032297	-0.014918	0.005938	52.03778	0.135449	-0.046728
368.5101	0.094244	-0.044933	0.018021	26.01682	0.268221	-0.092136
177.8099	0.212851	-0.106536	0.043028	13.25155	0.361412	-0.118863
89.06562	0.341602	-0.182594	0.075024	6.831852	0.292908	-0.061200
45.85412	0.326762	-0.166175	0.066701	3.482355	0.107504	0.150085
23.80629	0.142869	0.093638	-0.057725	1.719432	0.012762	0.361382
12.22564	0.018858	0.458613	-0.261829	0.810926	0.001220	0.394546
6.365056	0.000980	0.453981	-0.295512	0.362726	0.000319	0.253116
3.233863	-0.000122	0.127351	0.152496	0.148255	0.000124	0.071184
1.609860	0.000003	0.006283	0.562576			
0.760490	-0.000051	0.001426	0.417721			
0.322298	0.000003	-0.000076	0.076578			

Table XLVIII. Ag 2S (26s16p13d) basis set. Energy(E_H) = -5197.698071

Exponent	s space					
	1s	2s	3s	4s	5s	
	-913.834870	-134.877680	-25.917092	-4.000821	-0.219711	
112846900.	0.000001	0.000000	0.000000	0.000000	0.000000	
16959820.	0.000005	-0.000002	0.000001	0.000000	0.000000	
3877170.	0.000026	-0.000008	0.000004	-0.000002	0.000000	
1102756.	0.000110	-0.000035	0.000015	-0.000006	0.000001	
360988.9	0.000401	-0.000129	0.000056	-0.000023	0.000005	
130655.5	0.001307	-0.000422	0.000183	-0.000076	0.000016	
51045.50	0.003911	-0.001265	0.000549	-0.000229	0.000048	
21197.48	0.010849	-0.003535	0.001536	-0.000639	0.000134	
9258.205	0.027925	-0.009238	0.004020	-0.001676	0.000351	
4219.809	0.065931	-0.022541	0.009857	-0.004105	0.000864	
1994.505	0.138615	-0.050556	0.022297	-0.009325	0.001955	
972.2558	0.243971	-0.101021	0.045403	-0.018999	0.004008	
486.4668	0.319231	-0.166331	0.077337	-0.032721	0.006855	
248.1980	0.250302	-0.183076	0.090556	-0.038492	0.008192	
127.4637	0.080376	-0.005408	0.002166	-0.001468	0.000147	
66.56795	0.004373	0.393841	-0.273816	0.126657	-0.026658	
35.32009	0.001082	0.527742	-0.522242	0.253583	-0.055324	
18.75558	-0.000544	0.217789	-0.182999	0.102403	-0.021358	
9.468980	0.000250	0.019882	0.628466	-0.447151	0.100490	
5.031817	-0.000189	0.000494	0.627427	-0.728049	0.184491	
2.482671	0.000098	-0.000098	0.107483	0.177409	-0.071805	
1.248204	-0.000044	-0.000098	0.000267	0.814891	-0.244267	
0.587131	0.000016	-0.000023	0.001927	0.399267	-0.240188	
0.152589	-0.000005	0.000000	-0.000222	0.020468	0.144877	
0.069830	0.000003	0.000000	0.000159	-0.007503	0.586673	
0.030737	-0.000001	0.000000	-0.000051	0.002105	0.414370	
	p space			d space		
Exponent	2p	3p	4p	Exponent	3d	4d
	-125.180840	-21.944698	-2.676161		-14.677463	-0.536833
64373.72	0.000039	-0.000018	0.000007	2080.460	0.000219	-0.000070
15240.49	0.000348	-0.000156	0.000062	629.1563	0.002125	-0.000682
4951.311	0.002015	-0.000909	0.000358	245.5741	0.012256	-0.003964
1895.713	0.008969	-0.004079	0.001609	109.0126	0.048054	-0.015629
805.7325	0.032298	-0.014917	0.005893	52.03778	0.135520	-0.044882
368.5101	0.094246	-0.044930	0.017876	26.01682	0.268349	-0.088551
177.8099	0.212855	-0.106530	0.042707	13.25155	0.361591	-0.114136
89.06562	0.341594	-0.182573	0.074395	6.831852	0.293062	-0.059093
45.85412	0.326756	-0.166146	0.066261	3.482355	0.107145	0.144339
23.80629	0.142878	0.093584	-0.057400	1.719432	0.012280	0.345310
12.22564	0.018861	0.458492	-0.259169	0.810926	0.000709	0.381935
6.365056	0.000981	0.454161	-0.293769	0.362726	-0.000037	0.270096
3.233863	-0.000122	0.127229	0.152154	0.148255	0.000024	0.107289
1.609860	0.000001	0.006354	0.550827			
0.760490	-0.000052	0.001479	0.420811			
0.322298	0.000001	-0.000010	0.087604			

Table XLIX. $\text{Ag } ^2S (26s16p14d)$ basis set. $\text{Energy}(E_H) = -5197.698177$

Exponent	s space					
	1s	2s	3s	4s	5s	
	-913.835460	-134.878280	-25.917687	-4.001368	-0.219971	
112846900.	0.000001	0.000000	0.000000	0.000000	0.000000	
16959820.	0.000005	-0.000002	0.000001	0.000000	0.000000	
3877170.	0.000026	-0.000008	0.000004	-0.000002	0.000000	
1102756.	0.000110	-0.000035	0.000015	-0.000006	0.000001	
360988.9	0.000401	-0.000129	0.000056	-0.000023	0.000005	
130655.5	0.001307	-0.000422	0.000183	-0.000076	0.000016	
51045.50	0.003911	-0.001265	0.000549	-0.000229	0.000048	
21197.48	0.010849	-0.003535	0.001536	-0.000639	0.000134	
9258.205	0.027925	-0.009238	0.004020	-0.001676	0.000352	
4219.809	0.065931	-0.022541	0.009857	-0.004106	0.000865	
1994.505	0.138615	-0.050556	0.022297	-0.009325	0.001956	
972.2558	0.243971	-0.101021	0.045403	-0.019000	0.004010	
486.4668	0.319231	-0.166331	0.077337	-0.032721	0.006859	
248.1980	0.250302	-0.183076	0.090556	-0.038493	0.008196	
127.4637	0.080376	-0.005408	0.002166	-0.001467	0.000148	
66.56795	0.004373	0.393841	-0.273816	0.126657	-0.026676	
35.32009	0.001082	0.527742	-0.522243	0.253589	-0.055349	
18.75558	-0.000544	0.217789	-0.182999	0.102400	-0.021380	
9.468980	0.000250	0.019882	0.628467	-0.447149	0.100566	
5.031817	-0.000189	0.000494	0.627426	-0.728069	0.184565	
2.482671	0.000098	-0.000098	0.107483	0.177422	-0.071796	
1.248204	-0.000044	-0.000098	0.000266	0.814913	-0.244493	
0.587131	0.000016	-0.000023	0.001927	0.399254	-0.240295	
0.152589	-0.000005	0.000000	-0.000222	0.020447	0.145307	
0.069830	0.000003	0.000000	0.000159	-0.007497	0.587118	
0.030737	-0.000001	0.000000	-0.000051	0.002111	0.413625	
	p space			d space		
Exponent	2p	3p	4p	Exponent	3d	4d
	-125.181440	-21.945292	-2.676682		-14.678054	-0.537263
64373.72	0.000039	-0.000018	0.000007	2080.460	0.000219	-0.000070
15240.49	0.000348	-0.000156	0.000062	629.1563	0.002125	-0.000682
4951.311	0.002015	-0.000909	0.000358	245.5741	0.012256	-0.003965
1895.713	0.008969	-0.004079	0.001609	109.0126	0.048053	-0.015623
805.7325	0.032298	-0.014917	0.005894	52.03778	0.135520	-0.044899
368.5101	0.094246	-0.044930	0.017876	26.01682	0.268348	-0.088498
177.8099	0.212855	-0.106530	0.042708	13.25155	0.361592	-0.114252
89.06562	0.341594	-0.182573	0.074396	6.831852	0.293059	-0.058836
45.85412	0.326756	-0.166147	0.066262	3.482355	0.107150	0.143840
23.80629	0.142878	0.093584	-0.057402	1.719432	0.012273	0.346224
12.22564	0.018861	0.458492	-0.259171	0.810926	0.000719	0.380226
6.365056	0.000981	0.454161	-0.293777	0.362726	-0.000050	0.273159
3.233863	-0.000122	0.127230	0.152161	0.148255	0.000040	0.101600
1.609860	0.000001	0.006353	0.550841	0.060620	-0.000013	0.006479
0.760490	-0.000052	0.001479	0.420814			
0.322298	0.000001	-0.000010	0.087577			

Table L. Cd 1S ($2s15p12d$) basis set. Energy(E_H) = -5465.132183

Exponent	s space				
	1s	2s	3s	4s	5s
	-955.315090	-142.006620	-27.708405	-4.450344	-0.264769
27930250.	0.000004	-0.000001	0.000001	0.000000	0.000000
4182130.	0.000030	-0.000010	0.000004	-0.000002	0.000000
951757.3	0.000160	-0.000052	0.000023	-0.000010	0.000002
269590.9	0.000677	-0.000218	0.000095	-0.000040	0.000010
87953.89	0.002461	-0.000796	0.000347	-0.000147	0.000035
31752.97	0.007978	-0.002593	0.001130	-0.000477	0.000113
12384.36	0.023384	-0.007707	0.003372	-0.001426	0.000339
5136.288	0.061710	-0.020937	0.009179	-0.003880	0.000922
2239.697	0.142148	-0.051543	0.022862	-0.009699	0.002308
1017.823	0.266249	-0.110176	0.049660	-0.021099	0.005017
478.3604	0.349355	-0.187959	0.088538	-0.038039	0.009073
229.4960	0.244014	-0.184748	0.092554	-0.040103	0.009557
105.7103	0.051444	0.115232	-0.067703	0.029951	-0.007137
53.99976	-0.003015	0.552563	-0.446617	0.214788	-0.052231
27.17038	0.002076	0.443979	-0.485928	0.249454	-0.061158
12.37030	-0.001234	0.075121	0.345014	-0.212577	0.053448
6.532001	0.000781	-0.007136	0.799412	-0.822892	0.229553
3.251896	-0.000418	0.003384	0.219041	-0.139039	0.025714
1.555973	0.000191	-0.001461	0.005853	0.868297	-0.307122
0.696184	-0.000062	0.000385	0.002168	0.511531	-0.308636
0.163024	0.000024	-0.000154	-0.000249	0.023072	0.261099
0.079844	-0.000018	0.000113	0.000198	-0.009763	0.598380
0.034237	0.000005	-0.000032	-0.000057	0.002214	0.314009

p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-132.046800	-23.597017	-3.053321		-16.071744	-0.763495
46585.73	0.000074	-0.000034	0.000013	1576.176	0.000451	-0.000153
11029.42	0.000658	-0.000298	0.000120	475.8501	0.004271	-0.001454
3581.949	0.003781	-0.001720	0.000689	185.3554	0.023344	-0.008021
1370.118	0.016473	-0.007582	0.003052	81.62631	0.084520	-0.029329
581.3028	0.056955	-0.026791	0.010802	38.59718	0.211144	-0.074523
265.2172	0.153327	-0.075322	0.030698	18.93769	0.349447	-0.119761
127.3043	0.300193	-0.156421	0.064299	9.456201	0.359684	-0.107302
63.37837	0.372316	-0.204607	0.085596	4.740035	0.176197	0.070564
32.18828	0.228238	-0.036095	0.003805	2.299348	0.028920	0.333970
16.11256	0.047815	0.363584	-0.202577	1.059116	0.001045	0.426322
8.206452	0.001180	0.531425	-0.349234	0.460285	0.000095	0.300284
4.171906	0.000559	0.212201	0.002100	0.181569	-0.000010	0.093636
2.034242	-0.000284	0.017961	0.538617			
0.938697	0.000039	0.001468	0.501563			
0.393934	-0.000024	0.000054	0.113478			

Table LI. Cd 1S ($23s15p12d$) basis set. Energy(E_H) = -5465.132245

s space						
Exponent	1s	2s	3s	4s	5s	
	-955.315070	-142.006550	-27.708332	-4.450277	-0.264685	
47107610.	0.000002	-0.000001	0.000000	0.000000	0.000000	
7053348.	0.000016	-0.000005	0.000002	-0.000001	0.000000	
1605166.	0.000083	-0.000027	0.000012	-0.000005	0.000001	
454683.4	0.000352	-0.000114	0.000050	-0.000021	0.000005	
148349.8	0.001284	-0.000414	0.000181	-0.000076	0.000018	
53562.99	0.004180	-0.001355	0.000591	-0.000250	0.000059	
20894.55	0.012398	-0.004045	0.001764	-0.000746	0.000178	
8668.687	0.033591	-0.011179	0.004897	-0.002070	0.000491	
3782.801	0.082084	-0.028343	0.012456	-0.005273	0.001257	
1721.883	0.173549	-0.065166	0.029048	-0.012318	0.002918	
812.3185	0.291999	-0.128198	0.058295	-0.024857	0.005943	
394.9012	0.330410	-0.195515	0.093513	-0.040187	0.009506	
195.5415	0.189069	-0.143795	0.073403	-0.032183	0.007845	
91.49079	0.030227	0.216998	-0.134729	0.061467	-0.015176	
47.16878	-0.002048	0.571849	-0.498496	0.241495	-0.057800	
24.18269	0.001185	0.359226	-0.389248	0.206092	-0.052642	
11.23966	-0.000689	0.047897	0.496345	-0.333308	0.089765	
5.880216	0.000381	-0.003492	0.739785	-0.815229	0.220921	
2.835935	-0.000199	0.001585	0.149012	0.056735	-0.021661	
1.401416	0.000095	-0.000786	-0.000056	0.875783	-0.339566	
0.635511	-0.000026	0.000157	0.002170	0.417781	-0.249149	
0.121298	0.000005	-0.000032	-0.000151	0.009401	0.615793	
0.043333	-0.000002	0.000012	0.000062	-0.002390	0.552007	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-132.046720	-23.596942	-3.053251		-16.071669	-0.763422
46577.47	0.000074	-0.000034	0.000013	1576.175	0.000451	-0.000153
11027.44	0.000658	-0.000298	0.000120	475.8457	0.004271	-0.001454
3581.295	0.003782	-0.001720	0.000689	185.3528	0.023345	-0.008021
1369.861	0.016478	-0.007584	0.003053	81.62451	0.084524	-0.029331
581.1899	0.056972	-0.026799	0.010806	38.59587	0.211155	-0.074527
265.1622	0.153368	-0.075344	0.030706	18.93694	0.349453	-0.119763
127.2760	0.300247	-0.156453	0.064313	9.455867	0.359676	-0.107297
63.36398	0.372309	-0.204601	0.085592	4.739895	0.176185	0.070570
32.18110	0.228163	-0.035989	0.003755	2.299363	0.028917	0.333960
16.10924	0.047780	0.363687	-0.202643	1.059106	0.001046	0.426352
8.205064	0.001179	0.531366	-0.349196	0.460278	0.000095	0.300254
4.171301	0.000558	0.212117	0.002179	0.181580	-0.000010	0.093636
2.034306	-0.000284	0.017950	0.538518			
0.938781	0.000038	0.001471	0.501622			
0.393949	-0.000024	0.000053	0.113491			

Table LII. Cd 1S ($24s16p13d$) basis set. Energy(E_H) = -5465.132768

s space						
Exponent	1s	2s	3s	4s	5s	
47947170.	-955.315240	-142.006740	-27.708533	-4.450456	-0.264819	
7179575.	0.000002	-0.000001	0.000000	0.000000	0.000000	
1634065.	0.000016	-0.000005	0.000002	-0.000001	0.000000	
462914.8	0.000082	-0.000026	0.000011	-0.000005	0.000001	
151049.2	0.000345	-0.000111	0.000048	-0.000020	0.000005	
54542.16	0.001255	-0.000405	0.000177	-0.000075	0.000018	
21278.03	0.004087	-0.001325	0.000578	-0.000244	0.000058	
8828.305	0.012124	-0.003955	0.001725	-0.000729	0.000173	
3852.628	0.032872	-0.010933	0.004789	-0.002024	0.000481	
1753.702	0.080451	-0.027747	0.012193	-0.005161	0.001227	
827.2767	0.170670	-0.063907	0.028474	-0.012076	0.002871	
402.0641	0.289130	-0.126283	0.057385	-0.024458	0.005825	
198.9561	0.331630	-0.194379	0.092813	-0.039892	0.009502	
93.23320	0.194276	-0.148484	0.075676	-0.033115	0.007934	
48.14298	0.032336	0.202687	-0.125018	0.056847	-0.013723	
24.68665	-0.002141	0.568169	-0.489292	0.236789	-0.057441	
11.49636	0.001280	0.372247	-0.406620	0.213921	-0.053073	
6.045115	-0.000752	0.052544	0.461372	-0.304306	0.078744	
2.956000	0.000432	-0.003976	0.753902	-0.815926	0.227208	
1.462527	-0.000234	0.001904	0.167366	-0.007903	-0.012703	
0.665937	0.000115	-0.000943	0.001021	0.868454	-0.314393	
0.159307	-0.000036	0.000227	0.002465	0.457288	-0.286830	
0.075151	0.000013	-0.000087	-0.000357	0.018291	0.301442	
0.032808	-0.000009	0.000062	0.000266	-0.007322	0.598198	
	0.000003	-0.000018	-0.000080	0.001764	0.277965	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
68276.85	-132.046930	-23.597146	-3.053430	2200.245	-16.071881	-0.763591
16161.38	0.000038	-0.000017	0.000007	665.3019	0.000217	-0.000074
5249.366	0.000339	-0.000153	0.000062	259.6815	0.002107	-0.000716
2009.491	0.001966	-0.000893	0.000358	115.3058	0.012178	-0.004175
854.0211	0.008762	-0.004009	0.001612	55.07584	0.047922	-0.016512
390.5973	0.031619	-0.014693	0.005913	27.56089	0.135562	-0.047626
188.5014	0.092563	-0.044386	0.017999	14.05894	0.269155	-0.094147
94.46112	0.210112	-0.105779	0.043202	7.265947	0.362848	-0.121577
48.66613	0.339733	-0.182652	0.075906	3.713175	0.291702	-0.059728
25.30282	0.328876	-0.169401	0.068902	1.839775	0.105069	0.158275
13.01518	0.146590	0.087566	-0.055679	0.870731	0.011733	0.366065
6.794815	0.019933	0.457025	-0.265277	0.390768	0.000651	0.390698
3.463262	0.000944	0.457400	-0.301433	0.160133	-0.000049	0.246337
1.725709	-0.000110	0.129658	0.154303		0.000022	0.068014
0.815609	-0.000015	0.006749	0.564314			
0.346387	-0.000050	0.001460	0.416649			
	0.000001	-0.000057	0.076471			

Table LIII. Cd 1S ($2s16p13d$) basis set. Energy(E_H) = -5465.132758

Exponent	s space				
	1s	2s	3s	4s	5s
	-955.315190	-142.006660	-27.708456	-4.450381	-0.264735
77119180.	0.000001	0.000000	0.000000	0.000000	0.000000
11542280.	0.000009	-0.000003	0.000001	-0.000001	0.000000
2626234.	0.000045	-0.000015	0.000006	-0.000003	0.000001
743850.6	0.000191	-0.000061	0.000027	-0.000011	0.000003
242691.9	0.000695	-0.000224	0.000098	-0.000041	0.000010
87627.34	0.002269	-0.000734	0.000320	-0.000135	0.000032
34184.00	0.006772	-0.002202	0.000961	-0.000406	0.000096
14183.08	0.018641	-0.006120	0.002672	-0.001130	0.000269
6190.043	0.047099	-0.015865	0.006960	-0.002941	0.000696
2818.620	0.106959	-0.037811	0.016677	-0.007071	0.001688
1330.529	0.207371	-0.081266	0.036434	-0.015453	0.003656
647.9399	0.310806	-0.146980	0.067624	-0.028943	0.006940
324.0699	0.297792	-0.195444	0.095110	-0.040911	0.009636
165.1684	0.133958	-0.088422	0.046098	-0.020627	0.005193
81.02690	0.015552	0.304123	-0.198716	0.092098	-0.022789
42.16425	-0.000302	0.564368	-0.523712	0.255629	-0.060963
21.97646	0.000210	0.290426	-0.297713	0.162777	-0.042867
10.59286	-0.000157	0.032395	0.576330	-0.405102	0.110377
5.562126	0.000045	-0.001132	0.685999	-0.783596	0.211231
2.684565	-0.000023	0.000547	0.122351	0.148535	-0.048335
1.338301	0.000014	-0.000367	-0.000513	0.858596	-0.341309
0.616968	-0.000003	0.000049	0.001973	0.382273	-0.231467
0.121361	0.000001	-0.000012	-0.000135	0.008405	0.617027
0.043308	0.000000	0.000005	0.000055	-0.002072	0.551600

p space			d space		
Exponent	2p	3p	4p	Exponent	3d
	-132.046850	-23.597068	-3.053355		-16.071802
68275.65	0.000038	-0.000017	0.000007	2199.706	0.000217
16160.13	0.000339	-0.000153	0.000062	665.1825	0.002107
5248.743	0.001967	-0.000893	0.000358	259.6443	0.012181
2009.191	0.008765	-0.004010	0.001612	115.2918	0.047930
853.8733	0.031628	-0.014698	0.005915	55.06998	0.135580
390.5219	0.092590	-0.044399	0.018005	27.55781	0.269185
188.4602	0.210168	-0.105810	0.043214	14.05703	0.362871
94.43703	0.339792	-0.182688	0.075922	7.264742	0.291675
48.65178	0.328844	-0.169359	0.068880	3.712393	0.105026
25.29422	0.146500	0.087760	-0.055774	1.839367	0.011721
13.01058	0.019901	0.457174	-0.265388	0.870512	0.000652
6.792484	0.000945	0.457248	-0.301307	0.390643	-0.000049
3.461995	-0.000111	0.129526	0.154574	0.160097	0.000022
1.725303	-0.000014	0.006733	0.564221		
0.815522	-0.000050	0.001461	0.416570		
0.346330	0.000002	-0.000057	0.076437		

Table LIV. Cd 1S (26s16p13d) basis set. Energy(E_H) = -5465.132858

s space						
Exponent	1s	2s	3s	4s	5s	
	-955.315280	-142.006750	-27.708546	-4.450467	-0.264820	
119397100.	0.000001	0.000000	0.000000	0.000000	0.000000	
17929520.	0.000005	-0.000002	0.000001	0.000000	0.000000	
4090629.	0.000026	-0.000008	0.000004	-0.000002	0.000000	
1161424.	0.000109	-0.000035	0.000015	-0.000006	0.000002	
379783.4	0.000397	-0.000128	0.000056	-0.000024	0.000006	
137407.8	0.001294	-0.000418	0.000182	-0.000077	0.000018	
53703.79	0.003867	-0.001253	0.000546	-0.000231	0.000055	
22320.38	0.010714	-0.003497	0.001527	-0.000644	0.000153	
9757.311	0.027561	-0.009130	0.003992	-0.001690	0.000402	
4449.958	0.065109	-0.022284	0.009794	-0.004139	0.000983	
2103.779	0.137137	-0.050035	0.022177	-0.009416	0.002243	
1025.571	0.242175	-0.100210	0.045261	-0.019214	0.004563	
513.1602	0.318770	-0.165619	0.077368	-0.033244	0.007941	
261.9303	0.252489	-0.184143	0.091511	-0.039440	0.009364	
134.7916	0.082786	-0.010477	0.004956	-0.002831	0.000797	
70.28461	0.004889	0.388693	-0.271157	0.127644	-0.031097	
37.29177	0.001007	0.530573	-0.526283	0.259304	-0.062762	
19.80800	-0.000506	0.222467	-0.192491	0.110767	-0.028814	
10.02245	0.000230	0.020516	0.629317	-0.460567	0.122761	
5.340537	-0.000178	0.000484	0.630758	-0.741436	0.205824	
2.643780	0.000092	-0.000120	0.109117	0.185966	-0.070751	
1.325516	-0.000040	-0.000094	0.000512	0.841410	-0.317863	
0.622341	0.000014	-0.000024	0.001849	0.378136	-0.253324	
0.159306	-0.000005	0.000001	-0.000228	0.013321	0.323137	
0.072531	0.000003	-0.000001	0.000162	-0.004651	0.606178	
0.031771	-0.000001	0.000000	-0.000049	0.001136	0.253812	
p space			d space			
Exponent	2p	3p	4p	Exponent	3d	4d
	-132.046940	-23.597155	-3.053437		-16.071889	-0.763598
68228.43	0.000038	-0.000017	0.000007	2198.852	0.000217	-0.000074
16149.98	0.000339	-0.000154	0.000062	664.9498	0.002109	-0.000717
5245.761	0.001968	-0.000894	0.000358	259.5628	0.012188	-0.004179
2008.147	0.008772	-0.004014	0.001613	115.2597	0.047951	-0.016522
853.4621	0.031650	-0.014708	0.005919	55.05639	0.135619	-0.047646
390.3453	0.092644	-0.044426	0.018016	27.55171	0.269221	-0.094169
188.3786	0.210255	-0.105857	0.043234	14.05433	0.362862	-0.121578
94.39801	0.339844	-0.182724	0.075939	7.263630	0.291618	-0.059656
48.63268	0.328765	-0.169281	0.068843	3.711965	0.104992	0.158391
25.28463	0.146385	0.087963	-0.055872	1.839230	0.011717	0.366085
13.00645	0.019870	0.457264	-0.265462	0.870508	0.000651	0.390654
6.790747	0.000946	0.457100	-0.301191	0.390667	-0.000049	0.246274
3.461238	-0.000112	0.129437	0.154738	0.160093	0.000022	0.067971
1.725016	-0.000014	0.006726	0.564208			
0.815453	-0.000050	0.001461	0.416449			
0.346369	0.000002	-0.000057	0.076451			

Table LV. In 2P ($24s19p13d$) basis set. Energy(E_H) = -5740.168848

Exponent	s space						
	1s	2s	3s	4s	5s		
	-997.800340	-149.395360	-29.624576	-4.976618	-0.372617		
51493990.	0.000002	-0.000001	0.000000	0.000000	0.000000		
7710802.	0.000015	-0.000005	0.000002	-0.000001	0.000000		
1754915.	0.000079	-0.000025	0.000011	-0.000005	0.000001		
497134.7	0.000332	-0.000107	0.000047	-0.000020	0.000005		
162208.7	0.001209	-0.000391	0.000171	-0.000073	0.000020		
58568.18	0.003939	-0.001279	0.000561	-0.000240	0.000065		
22846.94	0.011692	-0.003819	0.001674	-0.000717	0.000193		
9478.446	0.031742	-0.010563	0.004648	-0.001993	0.000537		
4135.967	0.077893	-0.026859	0.011858	-0.005088	0.001372		
1882.464	0.166160	-0.062053	0.027764	-0.011945	0.003220		
887.8256	0.284561	-0.123518	0.056353	-0.024342	0.006573		
431.2932	0.333315	-0.192853	0.092329	-0.040266	0.010877		
213.2556	0.202425	-0.155675	0.079595	-0.035242	0.009571		
100.3055	0.035877	0.180859	-0.111288	0.051102	-0.013991		
51.94195	-0.002249	0.561477	-0.478006	0.234683	-0.064626		
26.66578	0.001425	0.392274	-0.434567	0.230834	-0.064968		
12.50061	-0.000855	0.060378	0.411185	-0.270095	0.079284		
6.651609	0.000513	-0.004705	0.770771	-0.830477	0.263577		
3.336245	-0.000281	0.002311	0.197566	-0.085518	0.013225		
1.642922	0.000136	-0.001102	0.004614	0.864028	-0.357751		
0.760783	-0.000046	0.000287	0.002362	0.503083	-0.360232		
0.202412	0.000018	-0.000118	-0.000333	0.023147	0.336023		
0.099210	-0.000013	0.000081	0.000234	-0.008283	0.620674		
0.043685	0.000004	-0.000023	-0.000068	0.001866	0.256970		
		p space				d space	
Exponent	2p	3p	4p	5p	Exponent	3d	4d
	-139.171840	-25.374197	-3.507136	-0.197256		-17.589474	-1.063062
91599.65	0.000025	-0.000011	0.000005	-0.000001	2443.526	0.000192	-0.000069
21676.21	0.000219	-0.000100	0.000041	-0.000008	739.2032	0.001873	-0.000670
7040.514	0.001277	-0.000583	0.000239	-0.000048	288.6566	0.010926	-0.003938
2695.960	0.005758	-0.002643	0.001080	-0.000214	128.3453	0.043640	-0.015813
1146.829	0.021227	-0.009867	0.004050	-0.000808	61.42913	0.125815	-0.046455
525.2832	0.064717	-0.030834	0.012683	-0.002520	30.84047	0.256819	-0.094817
254.2369	0.158140	-0.078619	0.032693	-0.006541	15.80947	0.358107	-0.127112
128.0499	0.289761	-0.152724	0.064053	-0.012739	8.222699	0.303867	-0.073905
66.45617	0.351463	-0.194131	0.082823	-0.016706	4.248065	0.119494	0.142032
35.06771	0.227240	-0.052125	0.012335	-0.001900	2.134835	0.015606	0.365158
18.39995	0.057723	0.296696	-0.168378	0.034376	1.029435	0.000744	0.401705
9.764266	0.003064	0.513708	-0.336923	0.073029	0.473556	-0.000021	0.245443
5.211999	0.000633	0.280577	-0.120177	0.019334	0.198003	0.000011	0.059800
2.677734	-0.000297	0.043099	0.406399	-0.101295			
1.325136	0.000043	0.001850	0.557209	-0.158220			
0.625913	-0.000047	0.000485	0.233428	-0.053783			
0.216856	0.000011	-0.000032	0.015578	0.282747			
0.085308	-0.000005	0.000011	-0.001368	0.562380			
0.032998	0.000002	-0.000005	0.000530	0.305553			

Table LVI. In 2P ($24s19p13d$) basis set. Energy(E_H) = -5740.168834

s space							
Exponent	1s	2s	3s	4s	5s		
	-997.800300	-149.395300	-29.624516	-4.976560	-0.372536		
82479890.	0.000001	0.000000	0.000000	0.000000	0.000000		
12385500.	0.000008	-0.000003	0.000001	-0.000001	0.000000		
2820974.	0.000043	-0.000014	0.000006	-0.000003	0.000001		
799301.2	0.000183	-0.000059	0.000026	-0.000011	0.000003		
260828.3	0.000669	-0.000216	0.000095	-0.000041	0.000011		
94187.15	0.002184	-0.000707	0.000309	-0.000133	0.000036		
36747.23	0.006518	-0.002122	0.000931	-0.000399	0.000107		
15248.00	0.017954	-0.005900	0.002588	-0.001110	0.000300		
6655.252	0.045437	-0.015309	0.006747	-0.002892	0.000777		
3030.640	0.103539	-0.036560	0.016197	-0.006962	0.001885		
1430.759	0.202125	-0.078896	0.035518	-0.015280	0.004099		
696.8714	0.307076	-0.143883	0.066425	-0.028814	0.007836		
348.6552	0.301973	-0.195272	0.095253	-0.041574	0.011107		
177.7215	0.142571	-0.099012	0.051767	-0.023358	0.006634		
86.87489	0.017988	0.284932	-0.185578	0.087032	-0.024484		
45.29580	-0.000567	0.564628	-0.519454	0.257302	-0.069632		
23.63622	0.000367	0.307383	-0.325310	0.179423	-0.053478		
11.39558	-0.000245	0.036853	0.548629	-0.388447	0.120968		
6.030819	0.000100	-0.001647	0.702884	-0.807165	0.247829		
2.963996	-0.000052	0.000785	0.137837	0.100590	-0.036349		
1.485778	0.000028	-0.000474	0.000668	0.865021	-0.397193		
0.699055	-0.000007	0.000079	0.002052	0.412848	-0.287051		
0.156156	0.000001	-0.000018	-0.000157	0.010430	0.678803		
0.057622	-0.000001	0.000007	0.000055	-0.002245	0.526111		
						p space	
Exponent	2p	3p	4p	5p	Exponent	3d	4d
	-139.171780	-25.374136	-3.507077	-0.197196		-17.589413	-1.063000
91615.13	0.000025	-0.000011	0.000005	-0.000001	2443.517	0.000192	-0.000069
21679.67	0.000219	-0.000100	0.000041	-0.000008	739.1845	0.001873	-0.000670
7041.450	0.001277	-0.000583	0.000238	-0.000048	288.6437	0.010927	-0.003938
2696.217	0.005757	-0.002643	0.001080	-0.000214	128.3376	0.043645	-0.015815
1146.887	0.021227	-0.009867	0.004050	-0.000808	61.42468	0.125830	-0.046461
525.2837	0.064721	-0.030836	0.012684	-0.002520	30.83760	0.256849	-0.094827
254.2239	0.158160	-0.078630	0.032698	-0.006542	15.80758	0.358129	-0.127119
128.0380	0.289793	-0.152743	0.064061	-0.012741	8.221552	0.303843	-0.073877
66.44852	0.351468	-0.194133	0.082823	-0.016706	4.247386	0.119455	0.142093
35.06323	0.227206	-0.052073	0.012310	-0.001896	2.134535	0.015595	0.365169
18.39744	0.057699	0.296782	-0.168430	0.034390	1.029277	0.000744	0.401727
9.762640	0.003062	0.513747	-0.336959	0.073033	0.473450	-0.000021	0.245380
5.210712	0.000632	0.280490	-0.120028	0.019304	0.197969	0.000011	0.059765
2.676673	-0.000296	0.043044	0.406796	-0.101398			
1.324188	0.000043	0.001847	0.557286	-0.158285			
0.625274	-0.000047	0.000484	0.232999	-0.053461			
0.216195	0.000010	-0.000032	0.015488	0.284432			
0.085063	-0.000005	0.000011	-0.001373	0.561348			
0.033011	0.000002	-0.000005	0.000529	0.304634			

Table LVII. In $^2P(26s19p13d)$ basis set. Energy(E_H) = -5740.168938

Exponent	s space					Exponent	d space	
	1s	2s	3s	4s	5s		3d	4d
	-997.800380	-149.395370	-29.624588	-4.976629	-0.372619			
126972000.	0.000001	0.000000	0.000000	0.000000	0.000000	2441.315	0.000192	-0.000069
19081310.	0.000005	-0.000002	0.000001	0.000000	0.000000	738.6687	0.001876	-0.000671
4360668.	0.000025	-0.000008	0.000004	-0.000002	0.000000	288.4804	0.010938	-0.003942
1240540.	0.000106	-0.000034	0.000015	-0.000006	0.000002	128.2745	0.043679	-0.015828
406484.3	0.000383	-0.000124	0.000054	-0.000023	0.000006	61.39708	0.125901	-0.046487
147358.0	0.001246	-0.000403	0.000177	-0.000076	0.000020	30.82439	0.256934	-0.094857
57697.84	0.003717	-0.001206	0.000528	-0.000226	0.000061	15.80101	0.358153	-0.127122
24021.91	0.010281	-0.003360	0.001474	-0.000631	0.000170	8.218251	0.303745	-0.073792
10518.93	0.026421	-0.008757	0.003847	-0.001651	0.000445	4.245641	0.119352	0.142253
4805.473	0.062438	-0.021363	0.009433	-0.004043	0.001088	2.133630	0.015569	0.365246
2275.795	0.131949	-0.048004	0.021366	-0.009196	0.002484	1.028877	0.000743	0.401629
1111.435	0.235076	-0.096581	0.043787	-0.018854	0.005077	0.473296	-0.000022	0.245289
557.3111	0.315549	-0.161364	0.075553	-0.032895	0.008911	0.197895	0.000011	0.059713
285.4381	0.260021	-0.186164	0.092602	-0.040497	0.010904			
148.0315	0.092970	-0.031340	0.016414	-0.007894	0.002279			
76.78754	0.007248	0.360173	-0.247901	0.117872	-0.032592			
40.82806	0.000747	0.538269	-0.524293	0.261847	-0.071934			
21.74785	-0.000351	0.248719	-0.240375	0.137115	-0.040113			
10.93727	0.000148	0.026286	0.590786	-0.430874	0.130577			
5.869906	-0.000138	-0.000103	0.660442	-0.774510	0.245306			
2.960463	0.000073	0.000151	0.129879	0.115839	-0.055028			
1.491527	-0.000031	-0.000218	0.001843	0.850899	-0.367619			
0.712310	0.000012	0.000010	0.001995	0.419170	-0.320716			
0.202977	-0.000004	-0.000011	-0.000271	0.016998	0.361559			
0.095828	0.000003	0.000007	0.000176	-0.005141	0.626341			
0.042281	-0.000001	-0.000002	-0.000052	0.001190	0.233513			

Table LVIII. Sn 3P ($24s19p13d$) basis set. Energy(E_H) = -6022.931398

s space						d space		
Exponent	1s	2s	3s	4s	5s	Exponent	3d	4d
	-1041.223200	-156.977500	-31.598900	-5.512425	-0.476390			
55147190.	0.000002	-0.000001	0.000000	0.000000	0.000000	2677.279	0.000175	-0.000065
8256841.	0.000014	-0.000005	0.000002	-0.000001	0.000000	810.1227	0.001710	-0.000638
1878999.	0.000076	-0.000025	0.000011	-0.000005	0.000001	316.4460	0.010043	-0.003778
532241.5	0.000321	-0.000104	0.000046	-0.000020	0.000006	140.8370	0.040585	-0.015354
173653.2	0.001169	-0.000378	0.000166	-0.000072	0.000021	67.51597	0.118726	-0.045744
62698.59	0.003807	-0.001237	0.000545	-0.000237	0.000069	33.97994	0.247515	-0.095650
24457.99	0.011304	-0.003697	0.001628	-0.000707	0.000207	17.48583	0.353983	-0.131893
10146.82	0.030722	-0.010230	0.004521	-0.001966	0.000575	9.139097	0.312161	-0.084678
4427.589	0.075564	-0.026054	0.011554	-0.005025	0.001470	4.758864	0.130502	0.130821
2015.128	0.161995	-0.060356	0.027113	-0.011828	0.003460	2.416542	0.018911	0.366100
950.2734	0.280168	-0.120935	0.055390	-0.024244	0.007102	1.181938	0.000840	0.410333
461.4771	0.334513	-0.191243	0.091794	-0.040602	0.011902	0.553351	-0.000003	0.241853
228.0740	0.209988	-0.162013	0.083093	-0.037230	0.010969	0.233716	-0.000001	0.053424
107.7638	0.039502	0.160012	-0.098281	0.045540	-0.013530			
55.93620	-0.002278	0.553652	-0.466104	0.232055	-0.069395			
28.74940	0.001552	0.411235	-0.460096	0.246816	-0.075406			
13.59098	-0.000950	0.068837	0.358624	-0.233814	0.074428			
7.311333	0.000588	-0.005243	0.784301	-0.840136	0.290324			
3.743075	-0.000323	0.002660	0.230835	-0.161673	0.044124			
1.831511	0.000155	-0.001232	0.008994	0.855171	-0.387437			
0.861628	-0.000056	0.000342	0.002131	0.545496	-0.423775			
0.250112	0.000023	-0.000146	-0.000260	0.028488	0.338248			
0.124879	-0.000015	0.000098	0.000166	-0.008921	0.646536			
0.055217	0.000004	-0.000026	-0.000050	0.001934	0.258758			

Table LIX. Sn 3P (26s19p13d) basis set. Energy(E_H) = -6022.931486

Exponent	s space					p space		d space				
	1s	2s	3s	4s	5s	2p	3p	4p	5p	Exponent	3d	4d
	-1041.223300	-156.977520	-31.598911	-5.512435	-0.476392							
139059100.	0.000001	0.000000	0.000000	0.000000	0.000000	-146.489200	-27.208974	-3.968991	-0.265007	2673.399	0.000175	-0.000065
20895080.	0.000005	-0.000001	0.000001	0.000000	0.000000	97825.17	-0.000011	0.000004	-0.000001	808.9857	0.001715	-0.000640
4775566.	0.000024	-0.000008	0.000003	-0.000001	0.000000	23170.05	-0.000096	0.000040	-0.000009	316.0237	0.010069	-0.003788
1358240.	0.000099	-0.000032	0.000014	-0.000006	0.000002	7531.418	-0.000561	0.000234	-0.000055	140.6582	0.040671	-0.015386
444800.5	0.000360	-0.000117	0.000051	-0.000022	0.000007	2885.973	-0.002543	0.001058	-0.000246	67.43386	0.118919	-0.045821
161148.4	0.001173	-0.000380	0.000167	-0.000073	0.000021	1228.576	-0.009501	0.003971	-0.000929	33.93961	0.247765	-0.095742
63064.05	0.003503	-0.001138	0.000501	-0.000218	0.000064	563.1789	-0.029771	0.012470	-0.002902	17.46525	0.354082	-0.131917
26245.08	0.009699	-0.003173	0.001398	-0.000607	0.000177	272.8287	-0.076381	0.032341	-0.007582	9.128598	0.311900	-0.084444
11488.67	0.024972	-0.008279	0.003653	-0.001589	0.000465	137.5811	-0.150073	0.064097	-0.014937	4.753341	0.130192	0.131285
5247.097	0.059219	-0.020241	0.008976	-0.003901	0.001139	71.50320	-0.195582	0.085036	-0.020105	2.413813	0.018825	0.366292
2484.535	0.125971	-0.045651	0.020398	-0.008897	0.002607	37.81191	-0.064558	0.018762	-0.003724	1.180709	0.000837	0.410141
1213.413	0.227191	-0.092526	0.042086	-0.018374	0.005368	19.91955	0.279314	-0.162496	0.038964	0.552818	-0.000004	0.241528
608.6750	0.312181	-0.156801	0.073553	-0.032434	0.009533	10.60978	0.513754	-0.342466	0.087379	0.233510	0.000000	0.053290
312.1552	0.268626	-0.188103	0.093570	-0.041505	0.012126	5.691044	0.295931	-0.142291	0.028344			
162.4874	0.104573	-0.051482	0.027419	-0.012874	0.003940	2.948548	0.049249	0.391271	-0.116129			
83.70844	0.009943	0.331979	-0.225773	0.108382	-0.032543	1.476426	0.002133	0.566869	-0.193064			
44.53542	0.000497	0.544099	-0.520537	0.263436	-0.078578	0.711913	0.000536	0.243577	-0.068792			
23.73708	-0.000202	0.273971	-0.283888	0.161686	-0.051081	0.263077	-0.000053	0.017429	0.326413			
11.90060	0.000072	0.032331	0.549770	-0.399710	0.131778	0.108903	0.000016	-0.001241	0.567527			
6.435359	-0.000098	-0.000655	0.686386	-0.802763	0.277079	0.043722	-0.000008	0.000513	0.261059			
3.303031	0.000052	0.000426	0.152667	0.046592	-0.032012							
1.666889	-0.000022	-0.000342	0.003847	0.857326	-0.405445							
0.807741	0.000010	0.000047	0.002030	0.457676	-0.379033							
0.249458	-0.000003	-0.000025	-0.000283	0.021113	0.374248							
0.119780	0.000002	0.000016	0.000163	-0.005501	0.647298							
0.053235	-0.000001	-0.000004	-0.000049	0.001257	0.231618							

Table LX. Sb 4S ($24s19p13d$) basis set. Energy(E_H) = -6313.485029

Exponent	s space					Exponent	d space	
	1s	2s	3s	4s	5s		3d	4d
	-1085.588900	-164.757890	-33.636146	-6.063115	-0.581731			
59184080.	0.000002	-0.000001	0.000000	0.000000	0.000000	2909.456	0.000161	-0.000063
8857706.	0.000014	-0.000005	0.000002	0.000001	0.000000	880.5592	0.001585	-0.000614
2015037.	0.000073	-0.000024	0.000010	0.000005	0.000001	344.0465	0.009358	-0.003653
570598.3	0.000309	-0.000100	0.000044	0.000019	0.000006	153.2369	0.038190	-0.014999
186114.9	0.001127	-0.000365	0.000161	0.000071	0.000022	73.55931	0.113084	-0.045217
67179.99	0.003672	-0.001195	0.000529	0.000233	0.000072	37.09627	0.239889	-0.096435
26199.43	0.010912	-0.003573	0.001580	0.000695	0.000216	19.15096	0.350266	-0.136098
10866.55	0.029699	-0.009895	0.004391	0.001935	0.000601	10.05016	0.318420	-0.093641
4740.431	0.073243	-0.025249	0.011246	0.004954	0.001539	5.266307	0.139577	0.121995
2156.916	0.157839	-0.058665	0.026454	0.011696	0.003634	2.696971	0.021861	0.367577
1016.782	0.275700	-0.118344	0.054404	0.024117	0.007503	1.334830	0.000941	0.417396
493.5330	0.335453	-0.189490	0.091169	0.040874	0.012727	0.633481	0.000008	0.237680
243.8108	0.217507	-0.167964	0.086380	0.039159	0.012251	0.269229	-0.000011	0.048602
115.8003	0.043421	0.139190	-0.085332	-0.039855	-0.012577			
60.20711	-0.002213	0.544599	-0.453257	-0.228640	-0.072677			
30.97254	0.001658	0.429849	-0.483915	-0.262139	-0.085089			
14.77771	-0.001032	0.078137	0.304200	0.196017	0.066143			
8.021914	0.000652	-0.005547	0.795278	0.845713	0.311164			
4.166745	-0.000358	0.002951	0.265957	0.235662	0.077680			
2.027207	0.000172	-0.001342	0.013781	-0.843180	-0.408816			
0.967674	-0.000066	0.000395	0.001844	-0.584394	-0.481629			
0.301685	0.000028	-0.000171	-0.000168	-0.034129	0.329234			
0.152076	-0.000018	0.000111	0.000085	0.009250	0.674676			
0.067348	0.000005	-0.000028	-0.000032	-0.001972	0.265387			
		p space						
Exponent	2p	3p	4p	5p	Exponent	3d	4d	
	-154.003720	-29.106076	-4.444653	-0.334674		-20.798002	-1.687802	
105974.5	0.000022	-0.000010	0.000004	-0.000001	2909.456	0.000161	-0.000063	
25071.12	0.000197	-0.000091	0.000038	-0.000010	880.5592	0.001585	-0.000614	
8141.447	0.001148	-0.000530	0.000225	-0.000058	344.0465	0.009358	-0.003653	
3117.121	0.005191	-0.002409	0.001020	-0.000263	153.2369	0.038190	-0.014999	
1326.053	0.019245	-0.009037	0.003843	-0.000996	73.55931	0.113084	-0.045217	
607.5271	0.059233	-0.028477	0.012136	-0.003131	37.09627	0.239889	-0.096435	
294.2062	0.147180	-0.073745	0.031766	-0.008254	19.15096	0.350266	-0.136098	
148.3589	0.277035	-0.147011	0.063884	-0.016507	10.05016	0.318420	-0.093641	
77.11804	0.351682	-0.197004	0.087219	-0.022854	5.266307	0.139577	0.121995	
40.82024	0.244671	-0.077556	0.025679	-0.005950	2.696971	0.021861	0.367577	
21.56258	0.069789	0.261433	-0.155901	0.041578	1.334830	0.000941	0.417396	
11.51041	0.004493	0.513578	-0.347692	0.098637	0.633481	0.000008	0.237680	
6.195810	0.000743	0.311268	-0.164092	0.037951	0.269229	-0.000011	0.048602	
3.231003	-0.000360	0.055590	0.377479	-0.126417				
1.633671	0.000067	0.002433	0.576551	-0.221715				
0.801241	-0.000066	0.000585	0.251936	-0.082532				
0.312384	0.000019	-0.000072	0.019062	0.354186				
0.133469	-0.000009	0.000025	-0.001273	0.570171				
0.054812	0.000003	-0.000009	0.000376	0.237739				

Table LXI. Sb 4S (26s19p13d) basis set. Energy(E_H) = -6313.485117

Exponent	s space					Exponent	d space	
	1s	2s	3s	4s	5s		3d	4d
	-1085.589000	-164.757900	-33.636156	-6.063125	-0.581733			
153960800.	0.000001	0.000000	0.000000	0.000000	0.000000	2904.651	0.000162	-0.000063
23127130.	0.000004	-0.000001	0.000001	0.000000	0.000000	879.2076	0.001590	-0.000616
5280132.	0.000022	-0.000007	0.000003	-0.000001	0.000000	343.5531	0.009384	-0.003664
1500011.	0.000092	-0.000030	0.000013	-0.000006	0.000002	153.0293	0.038277	-0.015033
490764.0	0.000335	-0.000109	0.000048	-0.000021	0.000007	73.46425	0.113282	-0.045298
177676.2	0.001092	-0.000354	0.000157	-0.000069	0.000021	37.04980	0.240152	-0.096537
69494.01	0.003264	-0.001061	0.000469	-0.000207	0.000064	19.12731	0.350383	-0.136131
28906.62	0.009051	-0.002963	0.001312	-0.000577	0.000179	10.03813	0.318160	-0.093402
12647.45	0.023360	-0.007744	0.003432	-0.001512	0.000470	5.259995	0.139244	0.122492
5773.481	0.055630	-0.018989	0.008455	-0.003723	0.001155	2.693828	0.021761	0.367801
2732.530	0.119262	-0.043022	0.019291	-0.008522	0.002652	1.333397	0.000938	0.417187
1334.073	0.218142	-0.087953	0.040122	-0.017750	0.005507	0.632846	0.000007	0.237326
669.1926	0.307674	-0.151443	0.071127	-0.031747	0.009910	0.268974	-0.000011	0.048468
343.4905	0.277727	-0.189348	0.094125	-0.042316	0.013134			
179.2013	0.118516	-0.072367	0.038674	-0.018083	0.005807			
91.49173	0.013532	0.300344	-0.201567	0.097598	-0.031142			
48.68974	0.000136	0.547849	-0.513747	0.263154	-0.083432			
25.93345	0.000018	0.301789	-0.327981	0.186931	-0.062439			
12.94463	-0.000051	0.039712	0.503419	-0.364293	0.127764			
7.051564	-0.000024	-0.001402	0.711153	-0.827458	0.304456			
3.670124	0.000012	0.000804	0.178180	-0.023812	-0.004108			
1.852016	-0.000002	-0.000511	0.006297	0.860798	-0.435431			
0.908631	0.000003	0.000104	0.002024	0.494240	-0.433108			
0.299716	-0.000001	-0.000046	-0.000288	0.025642	0.372917			
0.145479	0.000000	0.000029	0.000141	-0.005685	0.670867			
0.064929	0.000000	-0.000007	-0.000046	0.001306	0.236933			

Table LXII. Te 3P ($24s19p13d$) basis set. Energy(E_H) = -6611.783762

Exponent	s space					p space		d space				
	1s	2s	3s	4s	5s	2p	3p	4p	5p	Exponent	3d	4d
	-1130.916900	-172.755330	-35.754816	-6.646947	-0.700513							
63218780.	0.000002	-0.000001	0.000000	0.000000	0.000000					3143.750	0.000151	-0.000060
9458888.	0.000013	-0.000004	0.000002	0.000001	0.000000					951.3403	0.001484	-0.000594
2151150.	0.000071	-0.000023	0.000010	0.000005	0.000001					371.7183	0.008807	-0.003554
608993.8	0.000299	-0.000097	0.000043	0.000019	0.000006					165.6474	0.036253	-0.014719
198597.5	0.001091	-0.000354	0.000157	0.000070	0.000023					79.60415	0.108478	-0.044828
71671.47	0.003557	-0.001159	0.000515	0.000230	0.000075					40.21160	0.233530	-0.097211
27945.56	0.010578	-0.003468	0.001540	0.000686	0.000224					20.81580	0.346974	-0.139913
11588.67	0.028823	-0.009609	0.004282	0.001911	0.000624					10.96162	0.323293	-0.101313
5054.680	0.071234	-0.024557	0.010984	0.004899	0.001601					5.773744	0.147140	0.114998
2299.626	0.154177	-0.057193	0.025885	0.011591	0.003789					2.977838	0.024465	0.369631
1083.904	0.271587	-0.116028	0.053534	0.024023	0.007864					1.488853	0.001041	0.423316
525.9901	0.335922	-0.187775	0.090563	0.041128	0.013473					0.714418	0.000014	0.233169
259.8225	0.224158	-0.172917	0.089172	0.040893	0.013462					0.304787	-0.000020	0.044251
124.0375	0.047233	0.120607	-0.073905	-0.034765	-0.011552							
64.56611	-0.002085	0.535208	-0.441004	-0.225272	-0.075368							
33.24771	0.001748	0.446076	-0.504083	-0.275797	-0.094274							
16.02645	-0.001103	0.087350	0.253319	0.160739	0.057015							
8.756116	0.000702	-0.005433	0.802819	0.848862	0.329057							
4.593037	-0.000386	0.003100	0.299614	0.301773	0.111235							
2.223181	0.000185	-0.001398	0.018698	-0.831410	-0.428309							
1.075342	-0.000074	0.000427	0.001476	-0.616853	-0.535855							
0.353467	0.000032	-0.000186	-0.000054	-0.039073	0.336799							
0.178341	-0.000019	0.000116	-0.000005	0.009228	0.698061							
0.078665	0.000005	-0.000029	-0.000014	-0.001993	0.260400							

Table LXIII. Te 3P (26s19p13d) basis set. Energy(E_H) = -6611.783850

Exponent	s space					Exponent	d space	
	1s	2s	3s	4s	5s		3d	4d
	-1130.916900	-172.755350	-35.754826	-6.646956	-0.700516			
161444400.	0.000001	0.000000	0.000000	0.000000	0.000000	3135.331	0.000151	-0.000061
24314750.	0.000004	-0.000001	0.000001	0.000000	0.000000	949.1879	0.001491	-0.000597
5568824.	0.000021	-0.000007	0.000003	-0.000001	0.000000	370.9887	0.008840	-0.003567
1586226.	0.000090	-0.000029	0.000013	-0.000006	0.000002	165.3559	0.036358	-0.014762
519923.4	0.000327	-0.000106	0.000047	-0.000021	0.000007	79.47513	0.108713	-0.044928
188465.8	0.001064	-0.000346	0.000153	-0.000068	0.000022	40.15001	0.233843	-0.097337
73782.63	0.003178	-0.001035	0.000459	-0.000205	0.000067	20.78483	0.347124	-0.139957
30714.48	0.008806	-0.002886	0.001283	-0.000572	0.000187	10.94585	0.323000	-0.101034
13447.71	0.022724	-0.007540	0.003355	-0.001497	0.000490	5.765337	0.146733	0.115633
6142.788	0.054151	-0.018489	0.008266	-0.003687	0.001203	2.973378	0.024331	0.370006
2909.276	0.116341	-0.041926	0.018875	-0.008442	0.002764	1.486610	0.001034	0.423100
1421.429	0.213887	-0.085941	0.039345	-0.017630	0.005754	0.713286	0.000014	0.232647
713.6360	0.304980	-0.148924	0.070161	-0.031699	0.010412	0.304254	-0.000020	0.044032
366.7156	0.281390	-0.189538	0.094407	-0.042997	0.014039			
191.5562	0.125313	-0.081799	0.043877	-0.020669	0.006970			
97.59391	0.015473	0.283799	-0.189975	0.092990	-0.031264			
52.00404	-0.000025	0.548022	-0.509796	0.264538	-0.088270			
27.71489	0.000125	0.316384	-0.352002	0.202466	-0.071211			
13.88420	-0.000112	0.044162	0.473139	-0.343951	0.127530			
7.615667	0.000014	-0.001605	0.724134	-0.844459	0.327714			
4.009286	-0.000009	0.000934	0.197468	-0.071887	0.018240			
2.025550	0.000009	-0.000572	0.008608	0.863249	-0.465383			
1.006847	-0.000002	0.000126	0.001937	0.518519	-0.479938			
0.350813	0.000001	-0.000054	-0.000277	0.029237	0.386113			
0.170526	0.000000	0.000033	0.000108	-0.005423	0.691023			
0.075810	0.000000	-0.000008	-0.000041	0.001297	0.231993			

Table LXIV. I^2P ($24s19p13d$) basis set. Energy(E_H) = -6917.980596

Exponent	s space					Exponent	d space	
	1s	2s	3s	4s	5s		3d	4d
	-1177.186200	-180.949150	-37.934397	-7.244293	-0.821074			
66832220.	0.000002	-0.000001	0.000000	0.000000	0.000000	3370.294	0.000143	-0.000059
10005430.	0.000013	-0.000004	0.000002	0.000001	0.000000	1020.426	0.001407	-0.000580
2276844.	0.000069	-0.000022	0.000010	0.000005	0.000002	398.8899	0.008380	-0.003482
644925.2	0.000292	-0.000095	0.000042	0.000019	0.000006	177.8745	0.034727	-0.014522
210418.1	0.001064	-0.000346	0.000154	0.000069	0.000024	85.57481	0.104802	-0.044601
75973.03	0.003468	-0.001131	0.000505	0.000228	0.000077	43.29332	0.228357	-0.098042
29636.13	0.010311	-0.003385	0.001509	0.000680	0.000231	22.46450	0.344188	-0.143422
12294.84	0.028102	-0.009375	0.004194	0.001894	0.000644	11.86531	0.327009	-0.107805
5364.624	0.069540	-0.023979	0.010768	0.004860	0.001654	6.276530	0.153219	0.109887
2441.348	0.151006	-0.055934	0.025407	0.011516	0.003919	3.256061	0.026639	0.372499
1150.960	0.267836	-0.113988	0.052781	0.023963	0.008167	1.642155	0.001125	0.428075
558.6389	0.335912	-0.186067	0.089966	0.041358	0.014107	0.794905	0.000016	0.227916
276.0995	0.229873	-0.176982	0.091511	0.042435	0.014546	0.339731	-0.000029	0.040507
132.6090	0.050941	0.103498	-0.063426	-0.030010	-0.010389			
69.08957	-0.001834	0.524928	-0.428609	-0.221550	-0.077213			
35.62646	0.001793	0.460913	-0.521431	-0.288057	-0.102584			
17.33980	-0.001144	0.097072	0.204147	0.126618	0.046631			
9.524484	0.000729	-0.005199	0.806983	0.848818	0.342989			
5.031862	-0.000401	0.003262	0.332889	0.364622	0.144958			
2.425929	0.000194	-0.001471	0.023901	-0.817569	-0.442080			
1.188518	-0.000081	0.000468	0.001052	-0.647105	-0.586209			
0.409836	0.000035	-0.000204	0.000074	-0.044474	0.333693			
0.206745	-0.000021	0.000123	-0.000100	0.009063	0.721813			
0.090944	0.000005	-0.000029	0.000004	-0.002010	0.262259			
	p space						d space	
Exponent	2p	3p	4p	5p	Exponent	3d	4d	
	-169.660280	-33.122242	-5.473295	-0.403139		-24.285622	-2.401143	
107415.1	0.000025	-0.000011	0.000005	-0.000001	3370.294	0.000143	-0.000059	
25420.58	0.000221	-0.000103	0.000045	-0.000013	1020.426	0.001407	-0.000580	
8256.888	0.001286	-0.000600	0.000262	-0.000077	398.8899	0.008380	-0.003482	
3161.774	0.005802	-0.002722	0.001190	-0.000350	177.8745	0.034727	-0.014522	
1345.068	0.021413	-0.010177	0.004464	-0.001317	85.57481	0.104802	-0.044601	
616.1943	0.065349	-0.031851	0.014027	-0.004130	43.29332	0.228357	-0.098042	
298.3281	0.159756	-0.081342	0.036180	-0.010707	22.46450	0.344188	-0.143422	
150.3445	0.292252	-0.158045	0.071136	-0.021003	11.86531	0.327009	-0.107805	
78.10421	0.351706	-0.198824	0.090676	-0.027026	6.276530	0.153219	0.109887	
41.25662	0.224072	-0.046041	0.009487	-0.001916	3.256061	0.026639	0.372499	
21.67175	0.055071	0.318327	-0.199293	0.061675	1.642155	0.001125	0.428075	
11.59642	0.002435	0.517948	-0.373905	0.121741	0.794905	0.000016	0.227916	
6.220919	0.000608	0.258702	-0.084219	0.013869	0.339731	-0.000029	0.040507	
3.255813	-0.000370	0.036202	0.468851	-0.184233				
1.666848	0.000081	0.002002	0.548817	-0.265413				
0.833854	-0.000068	0.000157	0.172119	-0.012852				
0.373603	0.000025	-0.000002	0.010513	0.435925				
0.161297	-0.000009	-0.000035	0.001447	0.528723				
0.066594	0.000003	-0.000002	0.000235	0.193544				

Table LXV. I^2P ($26s19p13d$) basis set. Energy(E_H) = -6917.980685

Exponent	s space					p space			d space			
	1s	2s	3s	4s	5s	2p	3p	4p	5p	Exponent	3d	4d
	-1177.186200	-180.949160	-37.934406	-7.244303	-0.821076							
172093800.	0.000001	0.000000	0.000000	0.000000	0.000000					3362.028	0.000143	-0.000059
25940750.	0.000004	-0.000001	0.000001	0.000000	0.000000					1018.029	0.001414	-0.000583
5944408.	0.000021	-0.000007	0.000003	-0.000001	0.000000					398.0002	0.008417	-0.003497
1693744.	0.000087	-0.000028	0.000013	-0.000006	0.000002					177.4973	0.034853	-0.014575
555277.4	0.000316	-0.000103	0.000046	-0.000021	0.000007					85.40161	0.105097	-0.044730
201313.1	0.001028	-0.000334	0.000149	-0.000067	0.000023					43.20914	0.228762	-0.098211
78822.56	0.003069	-0.001001	0.000446	-0.000201	0.000068					22.42204	0.344388	-0.143486
32814.89	0.008509	-0.002792	0.001246	-0.000562	0.000191					11.84400	0.326636	-0.107450
14367.65	0.021975	-0.007297	0.003260	-0.001471	0.000501					6.265542	0.152701	0.110655
6563.090	0.052455	-0.017910	0.008038	-0.003629	0.001233					3.250578	0.026470	0.372872
3108.440	0.113083	-0.040692	0.018388	-0.008321	0.002837					1.639644	0.001117	0.427726
1518.849	0.209273	-0.083743	0.038468	-0.017446	0.005928					0.793777	0.000015	0.227374
762.6216	0.302223	-0.146265	0.069095	-0.031580	0.010801					0.339260	-0.000029	0.040338
391.9603	0.285484	-0.189778	0.094693	-0.043657	0.014841							
204.7608	0.132668	-0.091225	0.049038	-0.023288	0.008160							
103.9976	0.017613	0.267312	-0.178415	0.088235	-0.030925							
55.49063	-0.000208	0.546998	-0.504950	0.265212	-0.092177							
29.60213	0.000248	0.331101	-0.374594	0.217396	-0.079637							
14.84875	-0.000185	0.049267	0.442894	-0.323465	0.125438							
8.203297	0.000063	-0.002088	0.734850	-0.858868	0.347799							
4.361956	-0.000036	0.001203	0.216936	-0.118486	0.041820							
2.205710	0.000023	-0.000698	0.011144	0.864456	-0.490745							
1.109556	-0.000007	0.000175	0.001809	0.541078	-0.522963							
0.405119	0.000003	-0.000072	-0.000259	0.033094	0.391567							
0.197045	-0.000002	0.000042	0.000069	-0.005098	0.710487							
0.087484	0.000000	-0.000010	-0.000036	0.001299	0.232103							

Table LXVI. Xe 1S (24s19p13d) basis set. Energy(E_H) = -7232.138065

Exponent	s space					p space				d space		
	1s	2s	3s	4s	5s	2p	3p	4p	5p	Exponent	3d	4d
	-1224.397700	-189.340060	-40.175601	-7.856242	-0.944377	-177.782380	-35.221600	-6.008282	-0.457254	3605.356	-26.118806	-2.777825
71082420.	0.000002	-0.000001	0.000000	0.000000	0.000000	0.000025	-0.000012	0.000005	-0.000002	1091.745	0.000135	-0.000057
10642320.	0.000013	-0.000004	0.000002	0.000001	0.000000	0.000226	-0.000106	0.000047	-0.000014	426.8530	0.001339	-0.000567
2421851.	0.000067	-0.000022	0.000010	0.000004	0.000002	0.001318	-0.000618	0.000274	-0.000084	190.4310	0.008001	-0.003413
686010.2	0.000283	-0.000092	0.000041	0.000019	0.000007	0.005944	-0.002803	0.001244	-0.000382	91.69956	0.033371	-0.014331
223823.9	0.001032	-0.000336	0.000150	0.000069	0.000024	0.021920	-0.010473	0.004662	-0.001433	46.45243	0.101518	-0.044358
80813.37	0.003366	-0.001099	0.000492	0.000225	0.000079	0.066787	-0.032740	0.014641	-0.004498	24.15487	0.223666	-0.098725
31524.33	0.010009	-0.003289	0.001473	0.000671	0.000236	0.162716	-0.083383	0.037653	-0.011609	12.79264	0.341554	-0.146590
13078.18	0.027302	-0.009113	0.004092	0.001869	0.000657	0.295767	-0.161109	0.073698	-0.022724	6.792993	0.158751	0.105112
5706.402	0.067684	-0.023340	0.010522	0.004802	0.001689	0.351416	-0.199483	0.092288	-0.028621	3.542693	0.028694	0.375026
2596.865	0.147551	-0.054555	0.024865	0.011400	0.004010	0.219140	-0.037771	0.004985	-0.000657	1.800995	0.001214	0.432159
1224.248	0.263723	-0.111744	0.051915	0.023832	0.008396	0.051827	0.333872	-0.214065	0.069757	0.878397	0.000016	0.223368
594.2007	0.335765	-0.184129	0.089222	0.041489	0.014631	0.002046	0.517746	-0.382977	0.129983	0.375917	-0.000037	0.037691
293.7987	0.236041	-0.181053	0.093826	0.043968	0.015579	0.000554	0.244714	-0.056510	0.004222			
141.9751	0.055183	0.085711	-0.052565	-0.024945	-0.008931	0.000362	0.031365	0.503356	-0.211844			
73.97328	-0.001481	0.513390	-0.415003	-0.216885	-0.078175	0.000081	0.001842	0.536794	-0.279141			
38.18805	0.001827	0.475624	-0.537683	-0.299665	-0.110357	-0.000067	0.000023	0.142771	0.030877			
18.78629	-0.001173	0.107789	0.153827	0.091500	0.034605	0.000027	0.000041	0.005881	0.463804			
10.34210	0.000744	-0.004439	0.809464	0.846259	0.353742	0.000010	-0.000032	0.001234	0.505645			
5.487182	-0.000410	0.003297	0.366506	0.426457	0.179461	0.000005	-0.000029	0.000020	-0.002031			
2.636719	0.000200	-0.001499	0.029385	-0.802417	-0.451607							
1.306924	-0.000087	0.000491	0.000585	-0.675767	-0.633548							
0.469391	0.000037	-0.000213	0.000210	-0.050084	0.327670							
0.236422	-0.000021	0.000125	-0.000197	0.008778	0.743969							
0.103898	0.000005	-0.000029	0.000020	-0.002031	0.265835							

Table LXVII. Xe 1S (26s19p13d) basis set. Energy(E_H) = -7232.138154

Exponent	s space					p space				d space		
	1s	2s	3s	4s	5s	2p	3p	4p	5p	Exponent	3d	4d
	-1224.397700	-189.340070	-40.175610	-7.856252	-0.944380	-177.782390	-35.221607	-6.008288	-0.457257		-26.118813	-2.777831
174332000.	0.000001	0.000000	0.000000	0.000000	0.000000	0.000026	-0.000012	0.000005	-0.000002	3595.747	0.000136	-0.000058
26391340.	0.000004	-0.000001	0.000001	0.000000	0.000000	0.000231	-0.000108	0.000048	-0.000015	1089.070	0.001345	-0.000570
6068091.	0.000021	-0.000007	0.000003	0.000001	0.000000	0.001344	-0.000630	0.000279	-0.000086	425.9012	0.008036	-0.003428
1734662.	0.000088	-0.000029	0.000013	0.000006	0.000002	0.006046	-0.002851	0.001265	-0.000388	190.0453	0.033484	-0.014379
570690.3	0.000319	-0.000104	0.000046	0.000021	0.000007	0.022244	-0.010630	0.004732	-0.001455	91.53068	0.101768	-0.044470
207641.2	0.001033	-0.000336	0.000151	0.000069	0.000024	0.067604	-0.033154	0.014829	-0.004556	46.37424	0.223990	-0.098865
81573.15	0.003071	-0.001002	0.000448	0.000205	0.000072	0.164191	-0.084191	0.038021	-0.011722	24.11713	0.341694	-0.146634
34060.33	0.008484	-0.002788	0.001249	0.000570	0.000200	0.297199	-0.162024	0.074139	-0.022863	12.77446	0.329903	-0.113481
14950.42	0.021853	-0.007265	0.003259	0.001487	0.000524	0.350879	-0.199039	0.092046	-0.028538	6.784026	0.158338	0.105696
6843.935	0.052060	-0.017795	0.008017	0.003661	0.001285	0.216826	-0.034321	0.003124	-0.000079	3.538439	0.028562	0.375266
3247.664	0.112085	-0.040364	0.018311	0.008380	0.002954	0.050602	0.338106	-0.216961	0.070755	1.799161	0.001207	0.431871
1589.767	0.207442	-0.082999	0.038268	0.017556	0.006166	0.001957	0.516653	-0.382595	0.129801	0.877610	0.000015	0.223006
799.7028	0.300406	-0.145096	0.068799	0.031797	0.011244	0.000532	0.241053	-0.050167	0.001892	0.375598	-0.000037	0.037592
411.8547	0.286242	-0.189386	0.094787	0.044220	0.015540	0.000353	0.030372	0.507133	-0.213684			
215.6107	0.135862	-0.095491	0.051541	0.024710	0.008947	0.000077	0.001836	0.533507	-0.277819			
109.6637	0.018840	0.257023	-0.171792	-0.085860	-0.031148	0.000064	0.000003	0.139788	0.034982			
58.65789	-0.000299	0.544909	-0.501260	-0.266518	-0.095805	0.000026	0.000047	0.005534	0.464783			
31.35363	0.000322	0.340536	-0.390495	-0.228948	-0.086801	0.000010	-0.000034	0.001261	0.503743			
15.82649	-0.000233	0.053096	0.416548	0.305714	0.123132	0.000003	0.000008	-0.000183	0.169345			
8.804276	0.000095	-0.002114	0.741889	0.870257	0.365017							
4.729494	-0.000055	0.001268	0.235933	0.161653	0.065258							
2.389812	0.000032	-0.000731	0.014114	-0.864876	-0.512983							
1.215630	-0.000012	0.000188	0.001548	-0.560894	-0.562282							
0.462439	0.000005	-0.000075	-0.000205	-0.036994	0.393559							
0.224774	-0.000003	0.000044	0.000011	0.004649	0.728999							
0.099834	0.000001	-0.000010	-0.000027	-0.001294	0.234176							

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