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HIGH-QUALITY GAUSSIAN BASIS SETS FOR FOURTH-ROW ATOMS

Harry Partridge and Knut Faegri, Jr.*
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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 4d and 5p 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 $5s^2 4d^n$ ground state configuration; Pd has $5s^0 4d^{n+2}$, and Nb, Mo, Ru, Rh, and Ag have $5s^1 4d^{n+1}$ ground states. For transition metal atoms, rather than using the ground states, we have chosen to use the lowest $5s^2 4d^n$ 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 $s^2 d^n$ 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 μE_H of the numerical results, and the 26 s sets have a maximum deviation of 284 μE_H (for Cd) and, for most sets, are within 250 μE_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 μE_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

	s space				
Exponent	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

	s space				
Exponent	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

	s space				
Exponent	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

	s space				
Exponent	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

	s space				
Exponent	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

	s space				
Exponent	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

	s space				
Exponent	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	3d	4d
	−83.478428	−13.019657	−1.487502	−7.515729	−0.336691
41213.72	0.000047	−0.000020	0.000007	0.000212	−0.000052
9755.642	0.000420	−0.000179	0.000062	0.002044	−0.000503
3168.514	0.002425	−0.001035	0.000360	0.011660	−0.002864
1212.532	0.010708	−0.004612	0.001607	0.044934	−0.011144
514.8240	0.038023	−0.016634	0.005807	0.125443	−0.031336
235.0797	0.108268	−0.048999	0.017213	0.248867	−0.062490
113.0855	0.234983	−0.111510	0.039432	0.343020	−0.081813
56.36324	0.355138	−0.180022	0.064572	0.313034	−0.065288
28.79582	0.307868	−0.138141	0.047683	0.149572	0.056410
14.72383	0.114118	0.141523	−0.068261	0.024460	0.273825
7.432949	0.011506	0.467991	−0.222059	0.000191	0.420912
3.761160	0.001232	0.425934	−0.238661	0.000340	0.357572
1.845680	−0.000197	0.111074	0.120909	−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

	s space				
Exponent	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

s space

Exponent	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

Exponent	2p	3p	4p
	−83.478460	−13.019689	−1.487532
41110.33	0.000047	−0.000020	0.000007
9732.583	0.000421	−0.000179	0.000062
3161.307	0.002434	−0.001039	0.000361
1209.800	0.010748	−0.004629	0.001613
513.6666	0.038154	−0.016693	0.005827
234.5528	0.108587	−0.049150	0.017267
112.8317	0.235477	−0.111763	0.039521
56.23698	0.355384	−0.180186	0.064637
28.73092	0.307361	−0.137613	0.047460
14.68876	0.113520	0.142806	−0.068787
7.415312	0.011373	0.468669	−0.222522
3.752355	0.001232	0.424983	−0.238056
1.840564	−0.000201	0.110278	0.122643
0.896035	0.000119	0.003172	0.531522
0.417676	−0.000061	0.001205	0.442905
0.174265	0.000014	−0.000236	0.086441

d space

Exponent	3d	4d
	−7.515761	−0.336722
1408.702	0.000213	−0.000052
425.5463	0.002049	−0.000504
165.8761	0.011684	−0.002870
73.44281	0.045002	−0.011161
34.88745	0.125574	−0.031370
17.33794	0.248989	−0.062518
8.749997	0.343015	−0.081806
4.429198	0.312877	−0.065227
2.202197	0.149420	0.056525
1.014658	0.024423	0.273882
0.448128	0.000191	0.420804
0.189725	0.000339	0.357510
0.074250	−0.000054	0.131911

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

	s space				
Exponent	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

s space

Exponent	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

Exponent	2p	3p	4p
	−94.599758	−15.442374	−1.857297
47638.24	0.000044	−0.000019	0.000007
11275.44	0.000390	−0.000169	0.000062
3661.925	0.002256	−0.000981	0.000359
1401.406	0.009998	−0.004384	0.001608
595.1657	0.035700	−0.015899	0.005842
271.8887	0.102642	−0.047244	0.017474
130.9236	0.226273	−0.109237	0.040680
65.36412	0.350230	−0.180563	0.068262
33.48602	0.315867	−0.149052	0.054637
17.22222	0.125133	0.122070	−0.064223
8.746748	0.014126	0.462943	−0.235035
4.470095	0.001161	0.438313	−0.260758
2.223903	−0.000163	0.118644	0.127583
1.093599	0.000082	0.004372	0.543898
0.512496	−0.000056	0.001262	0.436188
0.215183	0.000010	−0.000184	0.083459

d space

Exponent	3d	4d
	−9.438458	−0.469958
1606.556	0.000210	−0.000059
485.3496	0.002026	−0.000572
189.2169	0.011626	−0.003288
83.84253	0.045182	−0.012885
39.89246	0.126997	−0.036612
19.87089	0.252930	−0.073131
10.06666	0.348125	−0.095810
5.135102	0.309083	−0.069914
2.588562	0.137743	0.080304
1.233712	0.020980	0.309586
0.564722	0.000526	0.422434
0.247233	0.000215	0.316224
0.099485	−0.000011	0.101076

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

	s space				
Exponent	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

	s space				
Exponent	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

	s space				
Exponent	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

Exponent	2p	3p	4p
	−100.406020	−16.699507	−2.041161
50536.21	0.000043	−0.000019	0.000007
11967.00	0.000383	−0.000167	0.000063
3888.220	0.002215	−0.000971	0.000363
1488.616	0.009818	−0.004341	0.001624
632.4927	0.035095	−0.015760	0.005906
289.0989	0.101126	−0.046924	0.017705
139.3134	0.223826	−0.108962	0.041393
69.62306	0.348632	−0.181247	0.069941
35.71634	0.317827	−0.152383	0.057066
18.41228	0.128350	0.117019	−0.063614
9.377044	0.014955	0.462662	−0.241717
4.814127	0.001123	0.441008	−0.268244
2.407017	−0.000157	0.119808	0.135078
1.188443	0.000067	0.004679	0.548391
0.558457	−0.000056	0.001302	0.430692
0.235510	0.000009	−0.000164	0.081577

d space

Exponent	3d	4d
	−10.444567	−0.543908
1703.907	0.000210	−0.000062
514.9879	0.002029	−0.000600
200.8760	0.011654	−0.003461
89.07686	0.045408	−0.013586
42.43043	0.127891	−0.038748
21.16285	0.254963	−0.077387
10.74104	0.350476	−0.101383
5.497212	0.307023	−0.070549
2.785001	0.132342	0.091515
1.345691	0.019385	0.322013
0.624435	0.000572	0.420325
0.276924	0.000095	0.300761
0.112710	−0.000015	0.090793

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

s space

Exponent	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

Exponent	2p	3p	4p
	−106.402430	−18.012357	−2.241298
37452.67	0.000079	−0.000035	0.000013
8867.424	0.000701	−0.000309	0.000118
2879.737	0.004018	−0.001779	0.000676
1101.303	0.017438	−0.007813	0.002983
467.0261	0.059882	−0.027426	0.010478
212.9025	0.159384	−0.076226	0.029453
102.0290	0.306809	−0.155502	0.060460
50.68028	0.371135	−0.197724	0.078338
25.65502	0.218508	−0.023278	−0.001678
12.76996	0.043286	0.365714	−0.187544
6.425252	0.001257	0.523553	−0.320133
3.234748	0.000522	0.213430	−0.018652
1.548473	−0.000205	0.017841	0.516823
0.708724	0.000035	0.001036	0.518715
0.295218	−0.000018	0.000007	0.122181

d space

Exponent	3d	4d
	−11.505334	−0.568830
1293.718	0.000435	−0.000134
390.3421	0.004107	−0.001258
151.9384	0.022325	−0.006913
66.80366	0.080360	−0.025007
31.50704	0.201119	−0.063812
15.41194	0.336386	−0.103240
7.636638	0.362907	−0.102407
3.783916	0.201204	0.031212
1.783331	0.038956	0.291575
0.805861	0.001026	0.436544
0.345588	0.000471	0.341011
0.134969	−0.000038	0.115296

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

	s space				
Exponent	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

s space

Exponent	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

Exponent	2p	3p	4p
	−106.402610	−18.012534	−2.241451
53964.10	0.000042	−0.000018	0.000007
12777.14	0.000372	−0.000164	0.000062
4151.208	0.002151	−0.000951	0.000361
1589.315	0.009546	−0.004253	0.001621
675.3326	0.034201	−0.015476	0.005907
308.7154	0.098949	−0.046250	0.017776
148.8057	0.220424	−0.108107	0.041838
74.40483	0.346600	−0.181529	0.071389
38.20322	0.320773	−0.156591	0.059906
19.73278	0.132754	0.109746	−0.061830
10.07167	0.016082	0.461139	−0.247215
5.190393	0.001087	0.445301	−0.276612
2.607285	−0.000145	0.122317	0.139204
1.290891	0.000050	0.005124	0.553308
0.607645	−0.000054	0.001332	0.427015
0.256316	0.000007	−0.000139	0.079851

d space

Exponent	3d	4d
	−11.505516	−0.568967
1783.114	0.000215	−0.000066
539.0008	0.002083	−0.000639
210.2526	0.011971	−0.003690
93.23163	0.046668	−0.014479
44.41613	0.131274	−0.041330
22.15367	0.260432	−0.081924
11.24415	0.354701	−0.106489
5.760238	0.301956	−0.067536
2.920268	0.122560	0.111033
1.421136	0.016483	0.336772
0.661871	0.000762	0.412151
0.293433	0.000134	0.284893
0.119222	0.000034	0.084968

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

	s space				
Exponent	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

	s space				
Exponent	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

	p space			d space		
Exponent	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

s space

Exponent	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

Exponent	2p	3p	4p
	−112.562040	−19.355822	−2.440794
57530.00	0.000041	−0.000018	0.000007
13616.39	0.000361	−0.000160	0.000062
4422.374	0.002093	−0.000932	0.000360
1692.686	0.009303	−0.004175	0.001616
719.1553	0.033412	−0.015229	0.005904
328.7443	0.097025	−0.045664	0.017832
158.4952	0.217373	−0.107363	0.042219
79.29024	0.344683	−0.181795	0.072670
40.74685	0.323312	−0.160359	0.062482
21.08477	0.136776	0.103196	−0.060096
10.78344	0.017153	0.459843	−0.252207
5.576591	0.001049	0.449061	−0.283979
2.812798	−0.000133	0.124507	0.143216
1.395610	0.000033	0.005551	0.557014
0.657768	−0.000053	0.001365	0.423947
0.277777	0.000005	−0.000117	0.078600

d space

Exponent	3d	4d
	−12.595835	−0.611229
1875.259	0.000218	−0.000069
566.8808	0.002109	−0.000668
221.1622	0.012132	−0.003866
98.09731	0.047365	−0.015182
46.76144	0.133260	−0.043416
23.33859	0.263876	−0.085755
11.85644	0.357541	−0.111041
6.085112	0.298317	−0.065184
3.089591	0.116054	0.126296
1.512768	0.014715	0.347105
0.707977	0.000896	0.405580
0.314828	0.000161	0.272249
0.128190	0.000063	0.079502

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

s space

Exponent	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

Exponent	2p	3p	4p
	−112.562110	−19.355890	−2.440857
57298.74	0.000041	−0.000018	0.000007
13565.13	0.000363	−0.000161	0.000062
4406.598	0.002105	−0.000937	0.000362
1686.911	0.009354	−0.004198	0.001626
716.7974	0.033577	−0.015305	0.005934
327.7063	0.097425	−0.045861	0.017910
158.0112	0.218003	−0.107701	0.042352
79.05636	0.345046	−0.182041	0.072777
40.63015	0.322724	−0.159776	0.062208
21.02420	0.135958	0.104766	−0.060828
10.75402	0.016936	0.460784	−0.252902
5.562181	0.001049	0.447920	−0.283137
2.804901	−0.000139	0.123551	0.145398
1.391790	0.000035	0.005442	0.557398
0.656105	−0.000053	0.001363	0.422478
0.277099	0.000006	−0.000118	0.078009

d space

Exponent	3d	4d
	−12.595902	−0.611294
1872.137	0.000219	−0.000069
566.0036	0.002116	−0.000670
220.8417	0.012165	−0.003877
97.96214	0.047470	−0.015216
46.70007	0.133477	−0.043489
23.30930	0.264105	−0.085823
11.84247	0.357557	−0.111034
6.078660	0.298016	−0.064985
3.086637	0.115798	0.126593
1.511611	0.014665	0.347140
0.707639	0.000895	0.405351
0.314777	0.000161	0.272142
0.128183	0.000063	0.079492

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

s space

Exponent	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

p space

Exponent	2p	3p	4p
	−118.889610	−20.734559	−2.642679
41889.99	0.000076	−0.000034	0.000013
9918.000	0.000678	−0.000304	0.000119
3220.979	0.003893	−0.001748	0.000684
1231.930	0.016927	−0.007693	0.003026
522.5530	0.058338	−0.027099	0.010670
238.3204	0.156201	−0.075773	0.030163
114.3077	0.303364	−0.156027	0.062579
56.84749	0.371807	−0.201366	0.082239
28.82677	0.223602	−0.029928	0.001076
14.39071	0.045625	0.364730	−0.195736
7.287032	0.001214	0.527818	−0.336040
3.687892	0.000543	0.212514	−0.007703
1.784669	−0.000246	0.017803	0.529767
0.820709	0.000037	0.001273	0.509169
0.343083	−0.000021	0.000029	0.116832

d space

Exponent	3d	4d
	−13.720575	−0.657193
1427.756	0.000446	−0.000145
430.9161	0.004216	−0.001374
167.7932	0.022969	−0.007560
73.83290	0.082871	−0.027482
34.86864	0.206939	−0.069886
17.08266	0.343668	−0.112427
8.499527	0.361059	−0.105801
4.240431	0.187013	0.052166
2.030714	0.033329	0.316646
0.926612	0.001353	0.431784
0.399703	0.000496	0.317952
0.156696	0.000057	0.103181

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

Exponent	2p	3p	4p
	−118.889550	−20.734499	−2.642625
41868.28	0.000076	−0.000034	0.000013
9912.706	0.000679	−0.000304	0.000119
3219.271	0.003896	−0.001750	0.000685
1231.297	0.016941	−0.007699	0.003028
522.2931	0.058380	−0.027119	0.010678
238.2033	0.156293	−0.075820	0.030182
114.2512	0.303472	−0.156091	0.062606
56.81953	0.371786	−0.201348	0.082230
28.81266	0.223441	−0.029700	0.000970
14.38412	0.045549	0.364967	−0.195877
7.284053	0.001213	0.527710	−0.335987
3.686453	0.000541	0.212308	−0.007448
1.784433	−0.000245	0.017771	0.529693
0.820696	0.000037	0.001277	0.509146
0.343069	−0.000021	0.000028	0.116817

d space

Exponent	3d	4d
	−13.720516	−0.657135
1427.627	0.000446	−0.000146
430.8802	0.004217	−0.001374
167.7792	0.022973	−0.007562
73.82588	0.082885	−0.027487
34.86466	0.206969	−0.069897
17.08049	0.343690	−0.112435
8.498462	0.361041	−0.105789
4.239912	0.186974	0.052204
2.030534	0.033315	0.316664
0.926507	0.001354	0.431820
0.399648	0.000495	0.317893
0.156687	0.000057	0.103153

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

s space

Exponent	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

Exponent	2p	3p	4p
	−118.889750	−20.734696	−2.642797
60945.43	0.000040	−0.000018	0.000007
14426.45	0.000354	−0.000158	0.000062
4685.952	0.002051	−0.000919	0.000360
1793.772	0.009122	−0.004122	0.001618
762.2309	0.032810	−0.015057	0.005920
348.5167	0.095530	−0.045260	0.017925
168.0937	0.214952	−0.106893	0.042631
84.14585	0.343054	−0.182176	0.073886
43.28296	0.325189	−0.163444	0.064697
22.43610	0.140028	0.098036	−0.058809
11.49888	0.018056	0.459049	−0.257094
5.967303	0.001013	0.451796	−0.290160
3.021461	−0.000126	0.126119	0.147721
1.501876	0.000017	0.005938	0.560048
0.708719	−0.000052	0.001395	0.420802
0.299831	0.000004	−0.000096	0.077560

d space

Exponent	3d	4d
	−13.720719	−0.657295
1974.971	0.000219	−0.000071
597.0892	0.002121	−0.000691
232.9947	0.012216	−0.004008
103.3848	0.047787	−0.015765
49.31574	0.134578	−0.045185
24.63374	0.266368	−0.089110
12.52993	0.359698	−0.115117
6.444892	0.295369	−0.063068
3.278323	0.111219	0.139128
1.612745	0.013526	0.355041
0.757956	0.001027	0.399705
0.338099	0.000213	0.261890
0.137934	0.000089	0.074998

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

s space

Exponent	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

Exponent	2p	3p	4p
	−125.385430	−22.149014	−2.847218
30875.26	0.000141	−0.000063	0.000025
7312.175	0.001243	−0.000560	0.000221
2374.139	0.007036	−0.003194	0.001272
906.9794	0.029772	−0.013704	0.005437
383.9592	0.097039	−0.046189	0.018570
174.4242	0.233778	−0.117109	0.047144
83.05950	0.375661	−0.202401	0.083784
40.81030	0.324344	−0.149163	0.056654
20.01061	0.105893	0.206259	−0.112524
9.884051	0.005887	0.550604	−0.337946
4.940968	0.001304	0.349468	−0.171080
2.259630	−0.000529	0.046618	0.460779
1.016750	0.000146	−0.000202	0.586776
0.417689	−0.000057	0.000574	0.165152

d space

Exponent	3d	4d
	−14.879905	−0.705602
1077.717	0.000922	−0.000306
324.8328	0.008425	−0.002841
125.9607	0.042798	−0.014426
54.86532	0.140214	−0.048455
25.53386	0.298898	−0.102185
12.18655	0.398999	−0.130900
5.889268	0.279612	−0.026177
2.733241	0.068788	0.263040
1.221291	0.002624	0.448758
0.511466	0.001182	0.368280
0.192977	0.000030	0.133601

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

	s space				
Exponent	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		
Exponent	2p	3p	4p
	−125.385640	−22.149249	−2.847420
30833.54	0.000141	−0.000063	0.000025
7302.327	0.001246	−0.000561	0.000222
2370.946	0.007052	−0.003201	0.001275
905.7602	0.029835	−0.013733	0.005449
383.4411	0.097221	−0.046280	0.018606
174.1845	0.234109	−0.117287	0.047216
82.94279	0.375863	−0.202540	0.083846
40.75098	0.324009	−0.148749	0.056453
19.97766	0.105502	0.207310	−0.113058
9.867951	0.005815	0.550857	−0.338268
4.933135	0.001307	0.348478	−0.169951
2.256352	−0.000530	0.046330	0.461757
1.015309	0.000146	−0.000192	0.586130
0.417150	−0.000058	0.000570	0.164562

	d space	
Exponent	3d	4d
	−14.880183	−0.705793
1500.512	0.000449	−0.000150
452.9389	0.004246	−0.001421
176.3987	0.023172	−0.007827
77.65016	0.083743	−0.028534
36.69544	0.209098	−0.072502
17.99281	0.346527	−0.116542
8.969764	0.360233	−0.107019
4.486903	0.181410	0.061372
2.163768	0.031326	0.325819
0.991712	0.001619	0.429243
0.428961	0.000585	0.308824
0.168533	0.000118	0.098273

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

s space

Exponent	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

p space

Exponent	2p	3p	4p
	−125.385720	−22.149338	−2.847497
30838.74	0.000141	−0.000063	0.000025
7303.553	0.001246	−0.000561	0.000222
2371.342	0.007050	−0.003200	0.001275
905.9123	0.029827	−0.013729	0.005448
383.5080	0.097197	−0.046268	0.018602
174.2165	0.234064	−0.117263	0.047206
82.95849	0.375836	−0.202521	0.083838
40.75892	0.324055	−0.148804	0.056480
19.98202	0.105554	0.207170	−0.112988
9.870116	0.005824	0.550819	−0.338221
4.934235	0.001307	0.348609	−0.170114
2.256887	−0.000530	0.046372	0.461596
1.015553	0.000146	−0.000193	0.586240
0.417240	−0.000058	0.000570	0.164655

d space

Exponent	3d	4d
	−14.880286	−0.705865
2083.467	0.000218	−0.000073
629.9597	0.002119	−0.000708
245.8548	0.012223	−0.004118
109.1257	0.047950	−0.016237
52.08560	0.135310	−0.046680
26.03758	0.268099	−0.092096
13.26124	0.361381	−0.118870
6.837103	0.293058	−0.061330
3.485695	0.107687	0.149609
1.722271	0.012822	0.360773
0.812640	0.001226	0.394770
0.363334	0.000320	0.253809
0.148420	0.000124	0.071333

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

	s space				
Exponent	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

	s space				
Exponent	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

	s space				
Exponent	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

	p space			d space		
Exponent	2p	3p	4p	Exponent	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

	s space				
Exponent	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		
Exponent	2p	3p	4p
	−125.385950	−22.149531	−2.847669
94658.22	0.000020	−0.000009	0.000004
22401.41	0.000178	−0.000080	0.000032
7276.528	0.001038	−0.000468	0.000186
2786.677	0.004699	−0.002128	0.000844
1185.788	0.017465	−0.007999	0.003186
543.3686	0.054068	−0.025304	0.010089
263.1771	0.136061	−0.066204	0.026673
132.7417	0.262271	−0.134648	0.054598
68.97937	0.349034	−0.190241	0.078709
36.53901	0.263014	−0.102085	0.036466
19.35069	0.085697	0.205403	−0.113033
10.22626	0.007542	0.494019	−0.295893
5.458158	0.000842	0.365941	−0.222266
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

	d space	
Exponent	3d	4d
	−14.880457	−0.706005
2082.525	0.000219	−0.000073
629.6503	0.002121	−0.000709
245.7252	0.012236	−0.004122
109.0638	0.047998	−0.016253
52.05505	0.135415	−0.046716
26.02236	0.268219	−0.092136
13.25319	0.361446	−0.118876
6.832263	0.292947	−0.061216
3.482386	0.107513	0.150083
1.719484	0.012760	0.361348
0.811032	0.001221	0.394490
0.362824	0.000318	0.253156
0.148283	0.000124	0.071240

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

	s space				
Exponent	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

s space

Exponent	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

Exponent	2p	3p	4p
	−125.180840	−21.944698	−2.676161
64373.72	0.000039	−0.000018	0.000007
15240.49	0.000348	−0.000156	0.000062
4951.311	0.002015	−0.000909	0.000358
1895.713	0.008969	−0.004079	0.001609
805.7325	0.032298	−0.014917	0.005893
368.5101	0.094246	−0.044930	0.017876
177.8099	0.212855	−0.106530	0.042707
89.06562	0.341594	−0.182573	0.074395
45.85412	0.326756	−0.166146	0.066261
23.80629	0.142878	0.093584	−0.057400
12.22564	0.018861	0.458492	−0.259169
6.365056	0.000981	0.454161	−0.293769
3.233863	−0.000122	0.127229	0.152154
1.609860	0.000001	0.006354	0.550827
0.760490	−0.000052	0.001479	0.420811
0.322298	0.000001	−0.000010	0.087604

d space

Exponent	3d	4d
	−14.677463	−0.536833
2080.460	0.000219	−0.000070
629.1563	0.002125	−0.000682
245.5741	0.012256	−0.003964
109.0126	0.048054	−0.015629
52.03778	0.135520	−0.044882
26.01682	0.268349	−0.088551
13.25155	0.361591	−0.114136
6.831852	0.293062	−0.059093
3.482355	0.107145	0.144339
1.719432	0.012280	0.345310
0.810926	0.000709	0.381935
0.362726	−0.000037	0.270096
0.148255	0.000024	0.107289

Table XLIX. Ag ^2S ($26s16p14d$) basis set. Energy(E_H) = −5197.698177

	s space				
Exponent	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 ($23s15p12d$) basis set. Energy(E_H) = −5465.132183

s space

Exponent	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

Exponent	2p	3p	4p
	−132.046800	−23.597017	−3.053321
46585.73	0.000074	−0.000034	0.000013
11029.42	0.000658	−0.000298	0.000120
3581.949	0.003781	−0.001720	0.000689
1370.118	0.016473	−0.007582	0.003052
581.3028	0.056955	−0.026791	0.010802
265.2172	0.153327	−0.075322	0.030698
127.3043	0.300193	−0.156421	0.064299
63.37837	0.372316	−0.204607	0.085596
32.18828	0.228238	−0.036095	0.003805
16.11256	0.047815	0.363584	−0.202577
8.206452	0.001180	0.531425	−0.349234
4.171906	0.000559	0.212201	0.002100
2.034242	−0.000284	0.017961	0.538617
0.938697	0.000039	0.001468	0.501563
0.393934	−0.000024	0.000054	0.113478

d space

Exponent	3d	4d
	−16.071744	−0.763495
1576.176	0.000451	−0.000153
475.8501	0.004271	−0.001454
185.3554	0.023344	−0.008021
81.62631	0.084520	−0.029329
38.59718	0.211144	−0.074523
18.93769	0.349447	−0.119761
9.456201	0.359684	−0.107302
4.740035	0.176197	0.070564
2.299348	0.028920	0.333970
1.059116	0.001045	0.426322
0.460285	0.000095	0.300284
0.181569	−0.000010	0.093636

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

Exponent	2p	3p	4p
	−132.046720	−23.596942	−3.053251
46577.47	0.000074	−0.000034	0.000013
11027.44	0.000658	−0.000298	0.000120
3581.295	0.003782	−0.001720	0.000689
1369.861	0.016478	−0.007584	0.003053
581.1899	0.056972	−0.026799	0.010806
265.1622	0.153368	−0.075344	0.030706
127.2760	0.300247	−0.156453	0.064313
63.36398	0.372309	−0.204601	0.085592
32.18110	0.228163	−0.035989	0.003755
16.10924	0.047780	0.363687	−0.202643
8.205064	0.001179	0.531366	−0.349196
4.171301	0.000558	0.212117	0.002179
2.034306	−0.000284	0.017950	0.538518
0.938781	0.000038	0.001471	0.501622
0.393949	−0.000024	0.000053	0.113491

d space

Exponent	3d	4d
	−16.071669	−0.763422
1576.175	0.000451	−0.000153
475.8457	0.004271	−0.001454
185.3528	0.023345	−0.008021
81.62451	0.084524	−0.029331
38.59587	0.211155	−0.074527
18.93694	0.349453	−0.119763
9.455867	0.359676	−0.107297
4.739895	0.176185	0.070570
2.299363	0.028917	0.333960
1.059106	0.001046	0.426352
0.460278	0.000095	0.300254
0.181580	−0.000010	0.093636

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

	s space				
Exponent	1s	2s	3s	4s	5s
	−955.315240	−142.006740	−27.708533	−4.450456	−0.264819
47947170.	0.000002	−0.000001	0.000000	0.000000	0.000000
7179575.	0.000016	−0.000005	0.000002	−0.000001	0.000000
1634065.	0.000082	−0.000026	0.000011	−0.000005	0.000001
462914.8	0.000345	−0.000111	0.000048	−0.000020	0.000005
151049.2	0.001255	−0.000405	0.000177	−0.000075	0.000018
54542.16	0.004087	−0.001325	0.000578	−0.000244	0.000058
21278.03	0.012124	−0.003955	0.001725	−0.000729	0.000173
8828.305	0.032872	−0.010933	0.004789	−0.002024	0.000481
3852.628	0.080451	−0.027747	0.012193	−0.005161	0.001227
1753.702	0.170670	−0.063907	0.028474	−0.012076	0.002871
827.2767	0.289130	−0.126283	0.057385	−0.024458	0.005825
402.0641	0.331630	−0.194379	0.092813	−0.039892	0.009502
198.9561	0.194276	−0.148484	0.075676	−0.033115	0.007934
93.23320	0.032336	0.202687	−0.125018	0.056847	−0.013723
48.14298	−0.002141	0.568169	−0.489292	0.236789	−0.057441
24.68665	0.001280	0.372247	−0.406620	0.213921	−0.053073
11.49636	−0.000752	0.052544	0.461372	−0.304306	0.078744
6.045115	0.000432	−0.003976	0.753902	−0.815926	0.227208
2.956000	−0.000234	0.001904	0.167366	−0.007903	−0.012703
1.462527	0.000115	−0.000943	0.001021	0.868454	−0.314393
0.665937	−0.000036	0.000227	0.002465	0.457288	−0.286830
0.159307	0.000013	−0.000087	−0.000357	0.018291	0.301442
0.075151	−0.000009	0.000062	0.000266	−0.007322	0.598198
0.032808	0.000003	−0.000018	−0.000080	0.001764	0.277965

	p space		
Exponent	2p	3p	4p
	−132.046930	−23.597146	−3.053430
68276.85	0.000038	−0.000017	0.000007
16161.38	0.000339	−0.000153	0.000062
5249.366	0.001966	−0.000893	0.000358
2009.491	0.008762	−0.004009	0.001612
854.0211	0.031619	−0.014693	0.005913
390.5973	0.092563	−0.044386	0.017999
188.5014	0.210112	−0.105779	0.043202
94.46112	0.339733	−0.182652	0.075906
48.66613	0.328876	−0.169401	0.068902
25.30282	0.146590	0.087566	−0.055679
13.01518	0.019933	0.457025	−0.265277
6.794815	0.000944	0.457400	−0.301433
3.463262	−0.000110	0.129658	0.154303
1.725709	−0.000015	0.006749	0.564314
0.815609	−0.000050	0.001460	0.416649
0.346387	0.000001	−0.000057	0.076471

	d space	
Exponent	3d	4d
	−16.071881	−0.763591
2200.245	0.000217	−0.000074
665.3019	0.002107	−0.000716
259.6815	0.012178	−0.004175
115.3058	0.047922	−0.016512
55.07584	0.135562	−0.047626
27.56089	0.269155	−0.094147
14.05894	0.362848	−0.121577
7.265947	0.291702	−0.059728
3.713175	0.105069	0.158275
1.839775	0.011733	0.366065
0.870731	0.000651	0.390698
0.390768	−0.000049	0.246337
0.160133	0.000022	0.068014

Table LIII. Cd ^1S ($24s16p13d$) basis set. Energy(E_H) = −5465.132758

	s space				
Exponent	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

s space

Exponent	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

Exponent	2p	3p	4p	5p
	−139.171840	−25.374197	−3.507136	−0.197256
91599.65	0.000025	−0.000011	0.000005	−0.000001
21676.21	0.000219	−0.000100	0.000041	−0.000008
7040.514	0.001277	−0.000583	0.000239	−0.000048
2695.960	0.005758	−0.002643	0.001080	−0.000214
1146.829	0.021227	−0.009867	0.004050	−0.000808
525.2832	0.064717	−0.030834	0.012683	−0.002520
254.2369	0.158140	−0.078619	0.032693	−0.006541
128.0499	0.289761	−0.152724	0.064053	−0.012739
66.45617	0.351463	−0.194131	0.082823	−0.016706
35.06771	0.227240	−0.052125	0.012335	−0.001900
18.39995	0.057723	0.296696	−0.168378	0.034376
9.764266	0.003064	0.513708	−0.336923	0.073029
5.211999	0.000633	0.280577	−0.120177	0.019334
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

d space

Exponent	3d	4d
	−17.589474	−1.063062
2443.526	0.000192	−0.000069
739.2032	0.001873	−0.000670
288.6566	0.010926	−0.003938
128.3453	0.043640	−0.015813
61.42913	0.125815	−0.046455
30.84047	0.256819	−0.094817
15.80947	0.358107	−0.127112
8.222699	0.303867	−0.073905
4.248065	0.119494	0.142032
2.134835	0.015606	0.365158
1.029435	0.000744	0.401705
0.473556	−0.000021	0.245443
0.198003	0.000011	0.059800

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				d 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

	s space				
Exponent	1s	2s	3s	4s	5s
	−997.800380	−149.395370	−29.624588	−4.976629	−0.372619
126972000.	0.000001	0.000000	0.000000	0.000000	0.000000
19081310.	0.000005	−0.000002	0.000001	0.000000	0.000000
4360668.	0.000025	−0.000008	0.000004	−0.000002	0.000000
1240540.	0.000106	−0.000034	0.000015	−0.000006	0.000002
406484.3	0.000383	−0.000124	0.000054	−0.000023	0.000006
147358.0	0.001246	−0.000403	0.000177	−0.000076	0.000020
57697.84	0.003717	−0.001206	0.000528	−0.000226	0.000061
24021.91	0.010281	−0.003360	0.001474	−0.000631	0.000170
10518.93	0.026421	−0.008757	0.003847	−0.001651	0.000445
4805.473	0.062438	−0.021363	0.009433	−0.004043	0.001088
2275.795	0.131949	−0.048004	0.021366	−0.009196	0.002484
1111.435	0.235076	−0.096581	0.043787	−0.018854	0.005077
557.3111	0.315549	−0.161364	0.075553	−0.032895	0.008911
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

	p space				d space		
Exponent	2p	3p	4p	5p	Exponent	3d	4d
	−139.171850	−25.374205	−3.507143	−0.197257		−17.589482	−1.063068
91677.91	0.000024	−0.000011	0.000005	−0.000001	2441.315	0.000192	−0.000069
21689.92	0.000219	−0.000100	0.000041	−0.000008	738.6687	0.001876	−0.000671
7043.256	0.001277	−0.000583	0.000238	−0.000048	288.4804	0.010938	−0.003942
2696.472	0.005757	−0.002643	0.001080	−0.000214	128.2745	0.043679	−0.015828
1146.863	0.021230	−0.009868	0.004051	−0.000809	61.39708	0.125901	−0.046487
525.2284	0.064737	−0.030844	0.012687	−0.002520	30.82439	0.256934	−0.094857
254.1823	0.158201	−0.078651	0.032706	−0.006544	15.80101	0.358153	−0.127122
128.0120	0.289850	−0.152776	0.064076	−0.012743	8.218251	0.303745	−0.073792
66.43271	0.351481	−0.194138	0.082823	−0.016707	4.245641	0.119352	0.142253
35.05342	0.227138	−0.051957	0.012253	−0.001882	2.133630	0.015569	0.365246
18.39124	0.057645	0.297000	−0.168560	0.034412	1.028877	0.000743	0.401629
9.758983	0.003055	0.513769	−0.336997	0.073051	0.473296	−0.000022	0.245289
5.208630	0.000632	0.280269	−0.119759	0.019224	0.197895	0.000011	0.059713
2.675960	−0.000296	0.042977	0.406893	−0.101395			
1.324061	0.000043	0.001851	0.557101	−0.158255			
0.625347	−0.000047	0.000482	0.232982	−0.053519			
0.216585	0.000011	−0.000032	0.015512	0.283360			
0.085196	−0.000005	0.000010	−0.001361	0.562362			
0.032964	0.000002	−0.000005	0.000528	0.304894			

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

s space

Exponent	1s	2s	3s	4s	5s
	−1041.223200	−156.977500	−31.598900	−5.512425	−0.476390
55147190.	0.000002	−0.000001	0.000000	0.000000	0.000000
8256841.	0.000014	−0.000005	0.000002	−0.000001	0.000000
1878999.	0.000076	−0.000025	0.000011	−0.000005	0.000001
532241.5	0.000321	−0.000104	0.000046	−0.000020	0.000006
173653.2	0.001169	−0.000378	0.000166	−0.000072	0.000021
62698.59	0.003807	−0.001237	0.000545	−0.000237	0.000069
24457.99	0.011304	−0.003697	0.001628	−0.000707	0.000207
10146.82	0.030722	−0.010230	0.004521	−0.001966	0.000575
4427.589	0.075564	−0.026054	0.011554	−0.005025	0.001470
2015.128	0.161995	−0.060356	0.027113	−0.011828	0.003460
950.2734	0.280168	−0.120935	0.055390	−0.024244	0.007102
461.4771	0.334513	−0.191243	0.091794	−0.040602	0.011902
228.0740	0.209988	−0.162013	0.083093	−0.037230	0.010969
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

p space

Exponent	2p	3p	4p	5p
	−146.489190	−27.208967	−3.968984	−0.265005
98883.58	0.000023	−0.000011	0.000004	−0.000001
23400.89	0.000206	−0.000094	0.000039	−0.000009
7600.878	0.001203	−0.000552	0.000230	−0.000054
2910.625	0.005434	−0.002508	0.001043	−0.000243
1238.269	0.020093	−0.009388	0.003924	−0.000918
567.2717	0.061584	−0.029472	0.012344	−0.002873
274.6544	0.151904	−0.075804	0.032095	−0.007524
138.4301	0.282601	−0.149418	0.063805	−0.014869
71.90813	0.351794	−0.195791	0.085138	−0.020128
38.01113	0.237193	−0.066737	0.019848	−0.003985
20.01874	0.064390	0.276573	−0.160886	0.038571
10.65700	0.003811	0.514002	−0.342248	0.087303
5.714510	0.000700	0.298357	−0.145282	0.029192
2.958781	−0.000332	0.050002	0.389180	−0.115564
1.481000	0.000056	0.002136	0.567916	−0.193207
0.713788	−0.000057	0.000549	0.245166	−0.069656
0.263564	0.000015	−0.000056	0.017609	0.325434
0.109106	−0.000007	0.000018	−0.001270	0.567760
0.043787	0.000002	−0.000008	0.000521	0.261964

d space

Exponent	3d	4d
	−19.163277	−1.368976
2677.279	0.000175	−0.000065
810.1227	0.001710	−0.000638
316.4460	0.010043	−0.003778
140.8370	0.040585	−0.015354
67.51597	0.118726	−0.045744
33.97994	0.247515	−0.095650
17.48583	0.353983	−0.131893
9.139097	0.312161	−0.084678
4.758864	0.130502	0.130821
2.416542	0.018911	0.366100
1.181938	0.000840	0.410333
0.553351	−0.000003	0.241853
0.233716	−0.000001	0.053424

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

	s space				
Exponent	1s	2s	3s	4s	5s
	−1041.223300	−156.977520	−31.598911	−5.512435	−0.476392
139059100.	0.000001	0.000000	0.000000	0.000000	0.000000
20895080.	0.000005	−0.000001	0.000001	0.000000	0.000000
4775566.	0.000024	−0.000008	0.000003	−0.000001	0.000000
1358240.	0.000099	−0.000032	0.000014	−0.000006	0.000002
444800.5	0.000360	−0.000117	0.000051	−0.000022	0.000007
161148.4	0.001173	−0.000380	0.000167	−0.000073	0.000021
63064.05	0.003503	−0.001138	0.000501	−0.000218	0.000064
26245.08	0.009699	−0.003173	0.001398	−0.000607	0.000177
11488.67	0.024972	−0.008279	0.003653	−0.001589	0.000465
5247.097	0.059219	−0.020241	0.008976	−0.003901	0.001139
2484.535	0.125971	−0.045651	0.020398	−0.008897	0.002607
1213.413	0.227191	−0.092526	0.042086	−0.018374	0.005368
608.6750	0.312181	−0.156801	0.073553	−0.032434	0.009533
312.1552	0.268626	−0.188103	0.093570	−0.041505	0.012126
162.4874	0.104573	−0.051482	0.027419	−0.012874	0.003940
83.70844	0.009943	0.331979	−0.225773	0.108382	−0.032543
44.53542	0.000497	0.544099	−0.520537	0.263436	−0.078578
23.73708	−0.000202	0.273971	−0.283888	0.161686	−0.051081
11.90060	0.000072	0.032331	0.549770	−0.399710	0.131778
6.435359	−0.000098	−0.000655	0.686386	−0.802763	0.277079
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

	p space				d space		
Exponent	2p	3p	4p	5p	Exponent	3d	4d
	−146.489200	−27.208974	−3.968991	−0.265007		−19.163285	−1.368982
97825.17	0.000024	−0.000011	0.000004	−0.000001	2673.399	0.000175	−0.000065
23170.05	0.000210	−0.000096	0.000040	−0.000009	808.9857	0.001715	−0.000640
7531.418	0.001222	−0.000561	0.000234	−0.000055	316.0237	0.010069	−0.003788
2885.973	0.005508	−0.002543	0.001058	−0.000246	140.6582	0.040671	−0.015386
1228.576	0.020332	−0.009501	0.003971	−0.000929	67.43386	0.118919	−0.045821
563.1789	0.062187	−0.029771	0.012470	−0.002902	33.93961	0.247765	−0.095742
272.8287	0.152989	−0.076381	0.032341	−0.007582	17.46525	0.354082	−0.131917
137.5811	0.283662	−0.150073	0.064097	−0.014937	9.128598	0.311900	−0.084444
71.50320	0.351475	−0.195582	0.085036	−0.020105	4.753341	0.130192	0.131285
37.81191	0.235514	−0.064558	0.018762	−0.003724	2.413813	0.018825	0.366292
19.91955	0.063411	0.279314	−0.162496	0.038964	1.180709	0.000837	0.410141
10.60978	0.003711	0.513754	−0.342466	0.087379	0.552818	−0.000004	0.241528
5.691044	0.000688	0.295931	−0.142291	0.028344	0.233510	0.000000	0.053290
2.948548	−0.000328	0.049249	0.391271	−0.116129			
1.476426	0.000054	0.002133	0.566869	−0.193064			
0.711913	−0.000056	0.000536	0.243577	−0.068792			
0.263077	0.000014	−0.000053	0.017429	0.326413			
0.108903	−0.000007	0.000016	−0.001241	0.567527			
0.043722	0.000002	−0.000008	0.000513	0.261059			

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

s space

Exponent	1s	2s	3s	4s	5s
	−1085.588900	−164.757890	−33.636146	−6.063115	−0.581731
59184080.	0.000002	−0.000001	0.000000	0.000000	0.000000
8857706.	0.000014	−0.000005	0.000002	0.000001	0.000000
2015037.	0.000073	−0.000024	0.000010	0.000005	0.000001
570598.3	0.000309	−0.000100	0.000044	0.000019	0.000006
186114.9	0.001127	−0.000365	0.000161	0.000071	0.000022
67179.99	0.003672	−0.001195	0.000529	0.000233	0.000072
26199.43	0.010912	−0.003573	0.001580	0.000695	0.000216
10866.55	0.029699	−0.009895	0.004391	0.001935	0.000601
4740.431	0.073243	−0.025249	0.011246	0.004954	0.001539
2156.916	0.157839	−0.058665	0.026454	0.011696	0.003634
1016.782	0.275700	−0.118344	0.054404	0.024117	0.007503
493.5330	0.335453	−0.189490	0.091169	0.040874	0.012727
243.8108	0.217507	−0.167964	0.086380	0.039159	0.012251
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
	−154.003720	−29.106076	−4.444653	−0.334674
105974.5	0.000022	−0.000010	0.000004	−0.000001
25071.12	0.000197	−0.000091	0.000038	−0.000010
8141.447	0.001148	−0.000530	0.000225	−0.000058
3117.121	0.005191	−0.002409	0.001020	−0.000263
1326.053	0.019245	−0.009037	0.003843	−0.000996
607.5271	0.059233	−0.028477	0.012136	−0.003131
294.2062	0.147180	−0.073745	0.031766	−0.008254
148.3589	0.277035	−0.147011	0.063884	−0.016507
77.11804	0.351682	−0.197004	0.087219	−0.022854
40.82024	0.244671	−0.077556	0.025679	−0.005950
21.56258	0.069789	0.261433	−0.155901	0.041578
11.51041	0.004493	0.513578	−0.347692	0.098637
6.195810	0.000743	0.311268	−0.164092	0.037951
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

d space

Exponent	3d	4d
	−20.798002	−1.687802
2909.456	0.000161	−0.000063
880.5592	0.001585	−0.000614
344.0465	0.009358	−0.003653
153.2369	0.038190	−0.014999
73.55931	0.113084	−0.045217
37.09627	0.239889	−0.096435
19.15096	0.350266	−0.136098
10.05016	0.318420	−0.093641
5.266307	0.139577	0.121995
2.696971	0.021861	0.367577
1.334830	0.000941	0.417396
0.633481	0.000008	0.237680
0.269229	−0.000011	0.048602

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

s space

Exponent	1s	2s	3s	4s	5s
	−1085.589000	−164.757900	−33.636156	−6.063125	−0.581733
153960800.	0.000001	0.000000	0.000000	0.000000	0.000000
23127130.	0.000004	−0.000001	0.000001	0.000000	0.000000
5280132.	0.000022	−0.000007	0.000003	−0.000001	0.000000
1500011.	0.000092	−0.000030	0.000013	−0.000006	0.000002
490764.0	0.000335	−0.000109	0.000048	−0.000021	0.000007
177676.2	0.001092	−0.000354	0.000157	−0.000069	0.000021
69494.01	0.003264	−0.001061	0.000469	−0.000207	0.000064
28906.62	0.009051	−0.002963	0.001312	−0.000577	0.000179
12647.45	0.023360	−0.007744	0.003432	−0.001512	0.000470
5773.481	0.055630	−0.018989	0.008455	−0.003723	0.001155
2732.530	0.119262	−0.043022	0.019291	−0.008522	0.002652
1334.073	0.218142	−0.087953	0.040122	−0.017750	0.005507
669.1926	0.307674	−0.151443	0.071127	−0.031747	0.009910
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

p space

Exponent	2p	3p	4p	5p
	−154.003730	−29.106084	−4.444659	−0.334676
104931.1	0.000022	−0.000010	0.000004	−0.000001
24842.42	0.000200	−0.000092	0.000039	−0.000010
8073.425	0.001164	−0.000537	0.000228	−0.000059
3093.292	0.005255	−0.002439	0.001032	−0.000266
1316.732	0.019450	−0.009135	0.003885	−0.001007
603.5788	0.059761	−0.028739	0.012249	−0.003160
292.4281	0.148163	−0.074269	0.031994	−0.008313
147.5200	0.278069	−0.147644	0.064170	−0.016582
76.71098	0.351509	−0.196897	0.087165	−0.022840
40.61595	0.243134	−0.075548	0.024657	−0.005677
21.45747	0.068796	0.264223	−0.157558	0.042029
11.45925	0.004371	0.513560	−0.348075	0.098766
6.169772	0.000735	0.308812	−0.161039	0.036990
3.219132	−0.000357	0.054739	0.379910	−0.127171
1.628189	0.000066	0.002420	0.575525	−0.221579
0.798901	−0.000065	0.000571	0.250106	−0.081430
0.311802	0.000019	−0.000068	0.018841	0.355247
0.133219	−0.000009	0.000023	−0.001240	0.569806
0.054729	0.000003	−0.000008	0.000367	0.236847

d space

Exponent	3d	4d
	−20.798009	−1.687808
2904.651	0.000162	−0.000063
879.2076	0.001590	−0.000616
343.5531	0.009384	−0.003664
153.0293	0.038277	−0.015033
73.46425	0.113282	−0.045298
37.04980	0.240152	−0.096537
19.12731	0.350383	−0.136131
10.03813	0.318160	−0.093402
5.259995	0.139244	0.122492
2.693828	0.021761	0.367801
1.333397	0.000938	0.417187
0.632846	0.000007	0.237326
0.268974	−0.000011	0.048468

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

s space

Exponent	1s	2s	3s	4s	5s
	−1130.916900	−172.755330	−35.754816	−6.646947	−0.700513
63218780.	0.000002	−0.000001	0.000000	0.000000	0.000000
9458888.	0.000013	−0.000004	0.000002	0.000001	0.000000
2151150.	0.000071	−0.000023	0.000010	0.000005	0.000001
608993.8	0.000299	−0.000097	0.000043	0.000019	0.000006
198597.5	0.001091	−0.000354	0.000157	0.000070	0.000023
71671.47	0.003557	−0.001159	0.000515	0.000230	0.000075
27945.56	0.010578	−0.003468	0.001540	0.000686	0.000224
11588.67	0.028823	−0.009609	0.004282	0.001911	0.000624
5054.680	0.071234	−0.024557	0.010984	0.004899	0.001601
2299.626	0.154177	−0.057193	0.025885	0.011591	0.003789
1083.904	0.271587	−0.116028	0.053534	0.024023	0.007864
525.9901	0.335922	−0.187775	0.090563	0.041128	0.013473
259.8225	0.224158	−0.172917	0.089172	0.040893	0.013462
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

p space

Exponent	2p	3p	4p	5p
	−161.734300	−31.083976	−4.952501	−0.359787
107544.8	0.000023	−0.000011	0.000005	−0.000001
25447.83	0.000206	−0.000095	0.000041	−0.000011
8264.421	0.001200	−0.000557	0.000240	−0.000067
3164.120	0.005421	−0.002529	0.001088	−0.000301
1345.920	0.020065	−0.009479	0.004096	−0.001139
616.5638	0.061571	−0.029798	0.012914	−0.003577
298.5425	0.152058	−0.076769	0.033618	−0.009376
150.5112	0.283109	−0.151562	0.067044	−0.018607
78.22458	0.352036	−0.198282	0.089185	−0.025084
41.37659	0.236667	−0.065686	0.019776	−0.004668
21.81310	0.063714	0.284208	−0.173494	0.049979
11.66666	0.003546	0.516773	−0.361029	0.110599
6.281730	0.000703	0.289889	−0.134878	0.030180
3.289850	−0.000378	0.047502	0.413936	−0.150016
1.677773	0.000079	0.002258	0.568071	−0.246667
0.836917	−0.000070	0.000413	0.220024	−0.058763
0.348285	0.000022	−0.000048	0.015832	0.396514
0.148014	−0.000009	−0.000001	0.000085	0.552044
0.060279	0.000003	−0.000006	0.000318	0.219431

d space

Exponent	3d	4d
	−22.512275	−2.038221
3143.750	0.000151	−0.000060
951.3403	0.001484	−0.000594
371.7183	0.008807	−0.003554
165.6474	0.036253	−0.014719
79.60415	0.108478	−0.044828
40.21160	0.233530	−0.097211
20.81580	0.346974	−0.139913
10.96162	0.323293	−0.101313
5.773744	0.147140	0.114998
2.977838	0.024465	0.369631
1.488853	0.001041	0.423316
0.714418	0.000014	0.233169
0.304787	−0.000020	0.044251

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

	s space				
Exponent	1s	2s	3s	4s	5s
	−1130.916900	−172.755350	−35.754826	−6.646956	−0.700516
161444400.	0.000001	0.000000	0.000000	0.000000	0.000000
24314750.	0.000004	−0.000001	0.000001	0.000000	0.000000
5568824.	0.000021	−0.000007	0.000003	−0.000001	0.000000
1586226.	0.000090	−0.000029	0.000013	−0.000006	0.000002
519923.4	0.000327	−0.000106	0.000047	−0.000021	0.000007
188465.8	0.001064	−0.000346	0.000153	−0.000068	0.000022
73782.63	0.003178	−0.001035	0.000459	−0.000205	0.000067
30714.48	0.008806	−0.002886	0.001283	−0.000572	0.000187
13447.71	0.022724	−0.007540	0.003355	−0.001497	0.000490
6142.788	0.054151	−0.018489	0.008266	−0.003687	0.001203
2909.276	0.116341	−0.041926	0.018875	−0.008442	0.002764
1421.429	0.213887	−0.085941	0.039345	−0.017630	0.005754
713.6360	0.304980	−0.148924	0.070161	−0.031699	0.010412
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

	p space				d space		
Exponent	2p	3p	4p	5p	Exponent	3d	4d
	−161.734310	−31.083983	−4.952507	−0.359790		−22.512282	−2.038227
106694.5	0.000023	−0.000011	0.000005	−0.000001	3135.331	0.000151	−0.000061
25255.40	0.000208	−0.000096	0.000041	−0.000011	949.1879	0.001491	−0.000597
8205.334	0.001214	−0.000563	0.000243	−0.000067	370.9887	0.008840	−0.003567
3142.962	0.005479	−0.002557	0.001100	−0.000304	165.3559	0.036358	−0.014762
1337.543	0.020256	−0.009570	0.004135	−0.001150	79.47513	0.108713	−0.044928
612.9816	0.062065	−0.030044	0.013022	−0.003607	40.15001	0.233843	−0.097337
296.9096	0.152984	−0.077267	0.033838	−0.009437	20.78483	0.347124	−0.139957
149.7277	0.284091	−0.152167	0.067323	−0.018686	10.94585	0.323000	−0.101034
77.83671	0.351854	−0.198153	0.089114	−0.025062	5.765337	0.146733	0.115633
41.17767	0.235210	−0.063644	0.018716	−0.004369	2.973378	0.024331	0.370006
21.70660	0.062801	0.287084	−0.175289	0.050517	1.486610	0.001034	0.423100
11.61283	0.003435	0.516624	−0.361301	0.110684	0.713286	0.000014	0.232647
6.253024	0.000697	0.287335	−0.131375	0.029011	0.304254	−0.000020	0.044032
3.276516	−0.000377	0.046653	0.416492	−0.150939			
1.671465	0.000079	0.002256	0.566766	−0.246395			
0.833974	−0.000069	0.000395	0.218014	−0.057315			
0.347637	0.000022	−0.000043	0.015600	0.397331			
0.147761	−0.000009	−0.000003	0.000117	0.551600			
0.060195	0.000003	−0.000005	0.000309	0.218686			

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

	s space				
Exponent	1s	2s	3s	4s	5s
	−1177.186200	−180.949150	−37.934397	−7.244293	−0.821074
66832220.	0.000002	−0.000001	0.000000	0.000000	0.000000
10005430.	0.000013	−0.000004	0.000002	0.000001	0.000000
2276844.	0.000069	−0.000022	0.000010	0.000005	0.000002
644925.2	0.000292	−0.000095	0.000042	0.000019	0.000006
210418.1	0.001064	−0.000346	0.000154	0.000069	0.000024
75973.03	0.003468	−0.001131	0.000505	0.000228	0.000077
29636.13	0.010311	−0.003385	0.001509	0.000680	0.000231
12294.84	0.028102	−0.009375	0.004194	0.001894	0.000644
5364.624	0.069540	−0.023979	0.010768	0.004860	0.001654
2441.348	0.151006	−0.055934	0.025407	0.011516	0.003919
1150.960	0.267836	−0.113988	0.052781	0.023963	0.008167
558.6389	0.335912	−0.186067	0.089966	0.041358	0.014107
276.0995	0.229873	−0.176982	0.091511	0.042435	0.014546
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

	s space				
Exponent	1s	2s	3s	4s	5s
	−1177.186200	−180.949160	−37.934406	−7.244303	−0.821076
172093800.	0.000001	0.000000	0.000000	0.000000	0.000000
25940750.	0.000004	−0.000001	0.000001	0.000000	0.000000
5944408.	0.000021	−0.000007	0.000003	−0.000001	0.000000
1693744.	0.000087	−0.000028	0.000013	−0.000006	0.000002
555277.4	0.000316	−0.000103	0.000046	−0.000021	0.000007
201313.1	0.001028	−0.000334	0.000149	−0.000067	0.000023
78822.56	0.003069	−0.001001	0.000446	−0.000201	0.000068
32814.89	0.008509	−0.002792	0.001246	−0.000562	0.000191
14367.65	0.021975	−0.007297	0.003260	−0.001471	0.000501
6563.090	0.052455	−0.017910	0.008038	−0.003629	0.001233
3108.440	0.113083	−0.040692	0.018388	−0.008321	0.002837
1518.849	0.209273	−0.083743	0.038468	−0.017446	0.005928
762.6216	0.302223	−0.146265	0.069095	−0.031580	0.010801
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

	p space				d space	
Exponent	2p	3p	4p	5p	Exponent	3d	4d
	−169.660290	−33.122249	−5.473301	−0.403142		−24.285629	−2.401149
106438.8	0.000025	−0.000012	0.000005	−0.000002	3362.028	0.000143	−0.000059
25204.46	0.000224	−0.000104	0.000045	−0.000013	1018.029	0.001414	−0.000583
8191.308	0.001304	−0.000608	0.000266	−0.000078	398.0002	0.008417	−0.003497
3138.324	0.005872	−0.002755	0.001204	−0.000354	177.4973	0.034853	−0.014575
1335.747	0.021640	−0.010286	0.004512	−0.001331	85.40161	0.105097	−0.044730
612.1937	0.065932	−0.032145	0.014158	−0.004168	43.20914	0.228762	−0.098211
296.5013	0.160828	−0.081925	0.036441	−0.010783	22.42204	0.344388	−0.143486
149.4681	0.293327	−0.158722	0.071456	−0.021100	11.84400	0.326636	−0.107450
77.66968	0.351377	−0.198560	0.090534	−0.026980	6.265542	0.152701	0.110655
41.03352	0.222389	−0.043574	0.008180	−0.001526	3.250578	0.026470	0.372872
21.55430	0.054128	0.321527	−0.201399	0.062361	1.639644	0.001117	0.427726
11.53606	0.002353	0.517396	−0.373879	0.121710	0.793777	0.000015	0.227374
6.187526	0.000594	0.255893	−0.079682	0.012270	0.339260	−0.000029	0.040338
3.238767	−0.000364	0.035358	0.471936	−0.185551			
1.658277	0.000079	0.001997	0.546770	−0.264792			
0.829139	−0.000067	0.000139	0.169581	−0.010287			
0.372324	0.000025	0.000003	0.010208	0.436944			
0.160839	−0.000009	−0.000037	0.001478	0.527683			
0.066451	0.000003	−0.000001	0.000225	0.192454			

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

	s space				
Exponent	1s	2s	3s	4s	5s
	−1224.397700	−189.340060	−40.175601	−7.856242	−0.944377
71082420.	0.000002	−0.000001	0.000000	0.000000	0.000000
10642320.	0.000013	−0.000004	0.000002	0.000001	0.000000
2421851.	0.000067	−0.000022	0.000010	0.000004	0.000002
686010.2	0.000283	−0.000092	0.000041	0.000019	0.000007
223823.9	0.001032	−0.000336	0.000150	0.000069	0.000024
80813.37	0.003366	−0.001099	0.000492	0.000225	0.000079
31524.33	0.010009	−0.003289	0.001473	0.000671	0.000236
13078.18	0.027302	−0.009113	0.004092	0.001869	0.000657
5706.402	0.067684	−0.023340	0.010522	0.004802	0.001689
2596.865	0.147551	−0.054555	0.024865	0.011400	0.004010
1224.248	0.263723	−0.111744	0.051915	0.023832	0.008396
594.2007	0.335765	−0.184129	0.089222	0.041489	0.014631
293.7987	0.236041	−0.181053	0.093826	0.043968	0.015579
141.9751	0.055183	0.085711	−0.052565	−0.024945	−0.008931
73.97328	−0.001481	0.513390	−0.415003	−0.216885	−0.078175
38.18805	0.001827	0.475624	−0.537683	−0.299665	−0.110357
18.78629	−0.001173	0.107789	0.153827	0.091500	0.034605
10.34210	0.000744	−0.004439	0.809464	0.846259	0.353742
5.487182	−0.000410	0.003297	0.366506	0.426457	0.179461
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

	p space				d space		
Exponent	2p	3p	4p	5p	Exponent	3d	4d
	−177.782380	−35.221600	−6.008282	−0.457254		−26.118806	−2.777825
110104.5	0.000025	−0.000012	0.000005	−0.000002	3605.356	0.000135	−0.000057
26056.61	0.000226	−0.000106	0.000047	−0.000014	1091.745	0.001339	−0.000567
8463.323	0.001318	−0.000618	0.000274	−0.000084	426.8530	0.008001	−0.003413
3240.730	0.005944	−0.002803	0.001244	−0.000382	190.4310	0.033371	−0.014331
1378.596	0.021920	−0.010473	0.004662	−0.001433	91.69956	0.101518	−0.044358
631.5261	0.066787	−0.032740	0.014641	−0.004498	46.45243	0.223666	−0.098725
305.7291	0.162716	−0.083383	0.037653	−0.011609	24.15487	0.341554	−0.146590
154.0567	0.295767	−0.161109	0.073698	−0.022724	12.79264	0.330220	−0.113769
80.02608	0.351416	−0.199483	0.092288	−0.028621	6.792993	0.158751	0.105112
42.25503	0.219140	−0.037771	0.004985	−0.000657	3.542693	0.028694	0.375026
22.17142	0.051827	0.333872	−0.214065	0.069757	1.800995	0.001214	0.432159
11.87360	0.002046	0.517746	−0.382977	0.129983	0.878397	0.000016	0.223368
6.356799	0.000554	0.244714	−0.056510	0.004222	0.375917	−0.000037	0.037691
3.321110	−0.000362	0.031365	0.503356	−0.211844			
1.703667	0.000081	0.001842	0.536794	−0.279141			
0.844142	−0.000067	0.000023	0.142771	0.030877			
0.397700	0.000027	0.000041	0.005881	0.463804			
0.175363	−0.000010	−0.000032	0.001234	0.505645			
0.073773	0.000003	0.000007	−0.000175	0.170795			

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

	s space				
Exponent	1s	2s	3s	4s	5s
	−1224.397700	−189.340070	−40.175610	−7.856252	−0.944380
174332000.	0.000001	0.000000	0.000000	0.000000	0.000000
26391340.	0.000004	−0.000001	0.000001	0.000000	0.000000
6068091.	0.000021	−0.000007	0.000003	0.000001	0.000000
1734662.	0.000088	−0.000029	0.000013	0.000006	0.000002
570690.3	0.000319	−0.000104	0.000046	0.000021	0.000007
207641.2	0.001033	−0.000336	0.000151	0.000069	0.000024
81573.15	0.003071	−0.001002	0.000448	0.000205	0.000072
34060.33	0.008484	−0.002788	0.001249	0.000570	0.000200
14950.42	0.021853	−0.007265	0.003259	0.001487	0.000524
6843.935	0.052060	−0.017795	0.008017	0.003661	0.001285
3247.664	0.112085	−0.040364	0.018311	0.008380	0.002954
1589.767	0.207442	−0.082999	0.038268	0.017556	0.006166
799.7028	0.300406	−0.145096	0.068799	0.031797	0.011244
411.8547	0.286242	−0.189386	0.094787	0.044220	0.015540
215.6107	0.135862	−0.095491	0.051541	0.024710	0.008947
109.6637	0.018840	0.257023	−0.171792	−0.085860	−0.031148
58.65789	−0.000299	0.544909	−0.501260	−0.266518	−0.095805
31.35363	0.000322	0.340536	−0.390495	−0.228948	−0.086801
15.82649	−0.000233	0.053096	0.416548	0.305714	0.123132
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

	p space				d space		
Exponent	2p	3p	4p	5p	Exponent	3d	4d
	−177.782390	−35.221607	−6.008288	−0.457257		−26.118813	−2.777831
108574.6	0.000026	−0.000012	0.000005	−0.000002	3595.747	0.000136	−0.000058
25721.71	0.000231	−0.000108	0.000048	−0.000015	1089.070	0.001345	−0.000570
8364.386	0.001344	−0.000630	0.000279	−0.000086	425.9012	0.008036	−0.003428
3206.235	0.006046	−0.002851	0.001265	−0.000388	190.0453	0.033484	−0.014379
1365.141	0.022244	−0.010630	0.004732	−0.001455	91.53068	0.101768	−0.044470
625.8338	0.067604	−0.033154	0.014829	−0.004556	46.37424	0.223990	−0.098865
303.1576	0.164191	−0.084191	0.038021	−0.011722	24.11713	0.341694	−0.146634
152.8321	0.297199	−0.162024	0.074139	−0.022863	12.77446	0.329903	−0.113481
79.42158	0.350879	−0.199039	0.092046	−0.028538	6.784026	0.158338	0.105696
41.94627	0.216826	−0.034321	0.003124	−0.000079	3.538439	0.028562	0.375266
22.01146	0.050602	0.338106	−0.216961	0.070755	1.799161	0.001207	0.431871
11.79188	0.001957	0.516653	−0.382595	0.129801	0.877610	0.000015	0.223006
6.311980	0.000532	0.241053	−0.050167	0.001892	0.375598	−0.000037	0.037592
3.298131	−0.000353	0.030372	0.507133	−0.213684			
1.692224	0.000077	0.001836	0.533507	−0.277819			
0.837469	−0.000064	0.000003	0.139788	0.034982			
0.395521	0.000026	0.000047	0.005534	0.464783			
0.174625	−0.000010	−0.000034	0.001261	0.503743			
0.073549	0.000003	0.000008	−0.000183	0.169345			

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Energy–optimized Gaussian basis sets of triple-zeta quality for the atoms Rb—Xe have been derived. Two series of basis sets are developed: (24*s* 16*p* 10*d*) and (26*s* 16*p* 10*d*) 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 (24*s* 16*p* 10*d*) 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 (26*s* 16*p* 10*d*) sets were derived. Total atomic energies from the largest basis sets are between 198 and 284 μE_H above the numerical Hartree-Fock energies.

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