WELL-TEMPERED GAUSSIAN BASIS SETS

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These basis sets were prepared using the new well-tempered formula introduced by S. Huzinaga and B. Miguel (Chem. Phys. Lett., **175** (1990) 289-291):

$$\begin{aligned} \zeta_N &= \alpha \\ \zeta_{N-k+1} &= \zeta_{N-k+2}\beta\left[1+\gamma\left(\tfrac{k}{N}\right)^{\delta}\right], \quad k=2,\ldots,N \end{aligned}$$

where α, β, γ, and δ are parameters (common for the radial functions of all angular symmetries) and N is the total number of exponential parameters generated by the formula. The parameters were optimized by minimizing the ground-state energy of an atom.

The additional parameter of the well-tempered basis sets, that is, the pattern in which of the primitives are shared between the s-, p-, d-, and f-spaces, can be deduced from the Tables. The Tables are numbered by the atomic number; for the atoms for which more than one basis set was prepared, the Table number is appended with the running basis set index.

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Z	Atom	State	N_s	N_p	N_d	N_f	Total Energy (in E_h)	Page
49	In	^2P	28	23	17		-5740.169018	81
50	Sn	^3P	28	23	17		-6022.931572	83
51	Sb	^4S	28	23	17		-6313.485205	85
52	Te	^3P	28	23	17		-6611.783948	87
53	I	^2P	28	23	17		-6917.980787	89
54	Xe	^1S	28	23	17		-7232.138256	91
55	Cs	^2S	30	23	17		-7553.933406	93
55	Cs	^2S	30	22	16		-7553.933344	95
56	Ba	^1S	30	23	17		-7883.543648	97
56	Ba	^1S	30	22	16		-7883.543542	99
57	La	^2F	30	23	17	14	-8221.063631	101
57	La	^2F	29	22	16	13	-8221.063495	103
58	Ce	^3H	30	23	17	14	-8566.919396	105
58	Ce	^3H	29	22	16	13	-8566.919256	107
59	Pr	^4I	30	23	17	14	-8921.180837	109
59	Pr	^4I	29	22	16	13	-8921.180691	111
60	Nd	^5I	30	23	17	14	-9283.882750	113
60	Nd	^5I	29	22	16	13	-9283.882591	115
61	Pm	^6H	30	23	17	14	-9655.098768	117
61	Pm	^6H	29	22	16	13	-9655.098597	119
62	Sm	^7F	30	23	17	14	-10034.95234	121
62	Sm	^7F	29	22	16	13	-10034.95216	123
63	Eu	^8S	30	23	17	14	-10423.54280	125
63	Eu	^8S	29	22	16	13	-10423.54261	127
64	Gd	^7F	30	23	17	14	-10820.61709	129
65	Tb	^6H	30	23	17	14	-11226.56814	131
66	Dy	^5I	29	22	16	13	-11641.45209	133
67	Ho	^4I	29	22	16	13	-12065.28927	135
68	Er	^3H	29	22	16	13	-12498.15221	137
69	Tm	^2F	29	22	16	13	-12940.17380	139
70	Yb	^1S	29	22	16	13	-13391.45555	141
71	Lu	^2D	28	21	18	12	-13851.80635	143
72	Hf	^3F	28	21	18	12	-14321.24839	145
73	Ta	^4F	28	21	18	12	-14799.81137	147
74	W	^5D	28	21	18	12	-15287.54525	149
75	Re	^6S	28	21	18	12	-15784.53216	151
76	Os	^5D	28	21	18	12	-16290.64760	153
77	Ir	^4F	28	21	18	12	-16806.11218	155
78	Pt	^3F	28	21	18	12	-17330.94853	157
79	Au	^2D	28	21	18	12	-17865.21057	159
80	Hg	^1S	29	21	19	13	-18408.99066	161
81	Tl	^2P	28	24	18	12	-18961.82286	163
82	Pb	^3P	28	24	18	12	-19524.00666	165
83	Bi	^4S	28	24	18	12	-20095.58511	167
84	Po	^3P	28	24	18	12	-20676.49965	169
85	At	^2P	28	24	18	12	-21266.88050	171
86	Rn	^1S	28	24	18	12	-21866.77108	173

For the **hydrogen atom**, we recommend the very accurate expansions prepared by Matsuoka *et al.* (*Bull. Univ. Electro-Comm.*, **2** (1989) 313; **5** (1992) 23) for use in molecular calculations in order to achieve balanced basis sets.

Table 2. He ^{1}S (17s; 17 ζ)

		Symmetry species	S
		Number of basis functions	17
Nuclear charge	2	Number of closed shells	1
No. of electrons	2	Open-shell occupation	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-2.861679975	-5.723359710	2.861679740	-2.00000008

	Orbital	1s
	Energy	-0.91796
ζ_1	279303.60	.0000003
ζ_2	53480.634	.0000020
ζ_3	12179.009	.0000116
ζ_4	3255.9044	.0000536
ζ_5	1005.0260	.0002080
ζ_6	351.28406	.0006927
ζ_7	136.10658	.0020459
ζ_8	57.213558	.0054969
ζ_9	25.571016	.0137224
ζ_{10}	11.938973	.0319305
ζ_{11}	5.7401136	.0683651
ζ_{12}	2.8110619	.1297721
ζ_{13}	1.3914291	.2108792
ζ_{14}	.69261487	.2804699
ζ_{15}	.34565755	.2725962
ζ_{16}	.17267382	.1380762
ζ_{17}	.08628295	.0194006

Table 3. Li ^{2}S (20s; 20 ζ)

		Symmetry species	S
		Number of basis functions	20
Nuclear charge	3	Number of closed shells	1
No. of electrons	3	Open-shell occupation	1

Coupling coefficients
$K_0^{ss} = -1.00000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-7.432726846	-14.86545240	7.432725550	-2.00000017

	Orbital	1s	2s
	Energy	-2.47774	-0.19632
ζ_1	483307.72	.0000005	-.0000001
ζ_2	90788.610	.0000031	-.0000005
ζ_3	20515.098	.0000177	-.0000028
ζ_4	5484.1328	.0000815	-.0000127
ζ_5	1699.6534	.0003136	-.0000490
ζ_6	597.02314	.0010376	-.0001622
ζ_7	232.15200	.0030510	-.0004780
ζ_8	97.686858	.0081917	-.0012863
ζ_9	43.583380	.0204005	-.0032296
ζ_{10}	20.267021	.0471582	-.0075570
ζ_{11}	9.6913182	.0988177	-.0162748
ζ_{12}	4.7178658	.1806869	-.0311066
ζ_{13}	2.3217784	.2734811	-.0519926
ζ_{14}	1.1496894	.3064735	-.0755494
ζ_{15}	.57116237	.1869768	-.0927545
ζ_{16}	.28419885	.0350450	-.0603857
ζ_{17}	.14150657	.0008334	.1077204
ζ_{18}	.07047515	.0001301	.4290474
ζ_{19}	.03510144	.0003908	.4763481
ζ_{20}	.01748314	.0000471	.1182689

Table 4. Be ^{1}S (20s; 20 ζ)

		Symmetry species	S
		Number of basis functions	20
Nuclear charge	4	Number of closed shells	2
No. of electrons	4	Open-shell occupation	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-14.57302299	-29.14604380	14.57302080	-2.00000015

	Orbital	1s	2s
	Energy	-4.73267	-0.30927
ζ_1	791926.49	.0000005	-.0000001
ζ_2	152594.32	.0000033	-.0000006
ζ_3	34946.426	.0000191	-.0000035
ζ_4	9374.5162	.0000881	-.0000161
ζ_5	2894.0932	.0003427	-.0000625
ζ_6	1007.9657	.0011499	-.0002098
ζ_7	387.83188	.0034331	-.0006276
ζ_8	161.49248	.0093269	-.0017118
ζ_9	71.405744	.0234161	-.0043380
ζ_{10}	32.981490	.0541828	-.0102161
ζ_{11}	15.702711	.1130445	-.0220662
ζ_{12}	7.6277240	.2036927	-.0423879
ζ_{13}	3.7522348	.2974348	-.0713885
ζ_{14}	1.8596241	.2966465	-.1016131
ζ_{15}	.92543781	.1392298	-.0951668
ζ_{16}	.46150028	.0155639	.0257675
ζ_{17}	.23035801	.0006867	.2466146
ζ_{18}	.11502470	-.0003878	.4397222
ζ_{19}	.05744160	.0001880	.3486851
ζ_{20}	.02868612	-.0000494	.0724784

Table 5. B ^{2}P (20s, 13p; 20 ζ)

		Symmetry species	S	P
		Number of basis functions	20	13
Nuclear charge	5	Number of closed shells	2	0
No. of electrons	5	Open-shell occupation	0	1

Coupling coefficients

$K_0^{pp} = -1.66666667$ $K_2^{pp} = 0.13333333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-24.52906021	-49.05812200	24.52906180	-1.99999993

	Orbital	1s	2s		2p
	Energy	-7.69534	-0.49471		-0.30986
ζ_1	1262544.2	.0000005	-.0000001		
ζ_2	250189.79	.0000031	-.0000006		
ζ_3	58235.632	.0000178	-.0000036		
ζ_4	15710.130	.0000820	-.0000166		
ζ_5	4833.6537	.0003226	-.0000652		
ζ_6	1665.9602	.0011042	-.0002233		
ζ_7	631.14318	.0033824	-.0006850		
ζ_8	257.95458	.0094464	-.0019230	ζ_8	.0000633
ζ_9	111.77932	.0244076	-.0050150	ζ_9	.0001315
ζ_{10}	50.578673	.0579583	-.0121685	ζ_{10}	.0006417
ζ_{11}	23.598284	.1235969	-.0269940	ζ_{11}	.0019936
ζ_{12}	11.240766	.2245007	-.0531508	ζ_{12}	.0062070
ζ_{13}	5.4263012	.3196586	-.0903379	ζ_{13}	.0165111
ζ_{14}	2.6407828	.2832028	-.1212639	ζ_{14}	.0415906
ζ_{15}	1.2911054	.1012119	-.0746815	ζ_{15}	.0979405
ζ_{16}	.63275517	.0065251	.1176195	ζ_{16}	.1941062
ζ_{17}	.31045529	.0009799	.3556490	ζ_{17}	.2929622
ζ_{18}	.15239109	-.0001691	.4415896	ζ_{18}	.3255305
ζ_{19}	.07481413	.0001849	.2194978	ζ_{19}	.2090497
ζ_{20}	.03673009	-.0000341	.0199809	ζ_{20}	.0489646

Table 6. C ^{3}P (20s, 13p; 20 ζ)

		Symmetry species	S	P
		Number of basis functions	20	13
Nuclear charge	6	Number of closed shells	2	0
No. of electrons	6	Open-shell occupation	0	2

Coupling coefficients

$K_0^{pp} = -0.66666667$ $K_2^{pp} = -0.06666667$

Total energy	Potential energy	Kinetic energy	Virial theorem
-37.68861796	-75.37724470	37.68862670	-1.99999977

	Orbital	1s	2s		2p
	Energy	-11.32552	-0.70563		-0.43334
ζ_1	2158490.7	.0000004	-.0000001		
ζ_2	429550.78	.0000025	-.0000005		
ζ_3	99951.327	.0000145	-.0000031		
ζ_4	26848.283	.0000672	-.0000143		
ζ_5	8199.1206	.0002678	-.0000571		
ζ_6	2798.3668	.0009306	-.0001986		
ζ_7	1048.2982	.0029000	-.0006195		
ζ_8	423.36984	.0082488	-.0017711	ζ_8	.0000591
ζ_9	181.26843	.0217501	-.0047105	ζ_9	.0001308
ζ_{10}	81.068295	.0528873	-.0116994	ζ_{10}	.0006373
ζ_{11}	37.403931	.1161595	-.0267177	ζ_{11}	.0020675
ζ_{12}	17.629539	.2182473	-.0544461	ζ_{12}	.0066669
ζ_{13}	8.4254263	.3215226	-.0953868	ζ_{13}	.0185913
ζ_{14}	4.0611964	.2942506	-.1290484	ζ_{14}	.0482527
ζ_{15}	1.9672294	.1090464	-.0740343	ζ_{15}	.1129009
ζ_{16}	.95541420	.0078308	.1342327	ζ_{16}	.2142291
ζ_{17}	.46459041	.0013767	.3701342	ζ_{17}	.3037437
ζ_{18}	.22603305	-.0001058	.4313976	ζ_{18}	.3111964
ζ_{19}	.10998858	.0002300	.2047999	ζ_{19}	.1846114
ζ_{20}	.05352300	-.0000391	.0182280	ζ_{20}	.0405258

Table 7. N ^{4}S (20s, 13p; 20 ζ)

		Symmetry species	S	P
		Number of basis functions	20	13
Nuclear charge	7	Number of closed shells	2	0
No. of electrons	7	Open-shell occupation	0	3

Coupling coefficients

$K_0^{pp} = -0.33333333$ $K_2^{pp} = -0.13333333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-54.40093246	-108.8019380	54.40100500	-1.99999868

	Orbital	1s	2s		2p
	Energy	-15.62905	-0.94532		-0.56759
ζ_1	3260308.3	.0000004	-.0000001		
ζ_2	666094.25	.0000021	-.0000005		
ζ_3	157037.16	.0000121	-.0000027		
ζ_4	42265.055	.0000566	-.0000125		
ζ_5	12820.260	.0002289	-.0000504		
ζ_6	4319.7754	.0008130	-.0001794		
ζ_7	1592.0629	.0025966	-.0005736		
ζ_8	631.83054	.0075704	-.0016805	ζ_8	.0000556
ζ_9	265.98991	.0204306	-.0045736	ζ_9	.0001326
ζ_{10}	117.17062	.0507643	-.0116072	ζ_{10}	.0006445
ζ_{11}	53.373044	.1138251	-.0270770	ζ_{11}	.0021697
ζ_{12}	24.896412	.2178873	-.0563381	ζ_{12}	.0071617
ζ_{13}	11.801350	.3248680	-.1001451	ζ_{13}	.0205499
ζ_{14}	5.6521249	.2972114	-.1341595	ζ_{14}	.0541283
ζ_{15}	2.7239663	.1089991	-.0689751	ζ_{15}	.1249247
ζ_{16}	1.3173740	.0081107	.1508479	ζ_{16}	.2280518
ζ_{17}	.63824304	.0015811	.3800553	ζ_{17}	.3078881
ζ_{18}	.30945957	-.0000194	.4206535	ζ_{18}	.2984467
ζ_{19}	.15008774	.0002337	.1923697	ζ_{19}	.1686927
ζ_{20}	.07279788	-.0000360	.0169242	ζ_{20}	.0362965

Table 8. O ^{3}P (20s, 13p; 20 ζ)

		Symmetry species	S	P
		Number of basis functions	20	13
Nuclear charge	8	Number of closed shells	2	0
No. of electrons	8	Open-shell occupation	0	4

Coupling coefficients

$K_0^{pp} = -0.16666667$ $K_2^{pp} = -0.01666667$

Total energy	Potential energy	Kinetic energy	Virial theorem
-74.80939527	-149.6190020	74.80960660	-1.99999718

	Orbital	1s	2s		2p
	Energy	-20.66862	-1.24430		-0.63189
ζ_1	4585516.2	.0000004	-.0000001		
ζ_2	925486.92	.0000020	-.0000005		
ζ_3	215772.29	.0000115	-.0000026		
ζ_4	57480.749	.0000545	-.0000124		
ζ_5	17270.167	.0002232	-.0000506		
ζ_6	5766.9282	.0008021	-.0001822		
ζ_7	2107.0076	.0025917	-.0005893		
ζ_8	829.06758	.0076418	-.0017468	ζ_8	.0000584
ζ_9	346.04791	.0208617	-.0048102	ζ_9	.0001446
ζ_{10}	151.12147	.0524042	-.0123557	ζ_{10}	.0007041
ζ_{11}	68.233250	.1186313	-.0291755	ζ_{11}	.0024243
ζ_{12}	31.542773	.2278800	-.0613291	ζ_{12}	.0081415
ζ_{13}	14.815300	.3348101	-.1090179	ζ_{13}	.0238707
ζ_{14}	7.0298236	.2885222	-.1394983	ζ_{14}	.0635884
ζ_{15}	3.3561489	.0928026	-.0491181	ζ_{15}	.1427596
ζ_{16}	1.6077662	.0058271	.1957403	ζ_{16}	.2435940
ζ_{17}	.77153240	.0014442	.4112333	ζ_{17}	.3049210
ζ_{18}	.37052330	.0001021	.3958343	ζ_{18}	.2805842
ζ_{19}	.17799002	.0001704	.1465890	ζ_{19}	.1571702
ζ_{20}	.08550795	-.0000190	.0089379	ζ_{20}	.0355116

Table 9. F ^{2}P (20s, 13p; 20 ζ)

		Symmetry species	S	P
		Number of basis functions	20	13
Nuclear charge	9	Number of closed shells	2	0
No. of electrons	9	Open-shell occupation	0	5

Coupling coefficients

$K_0^{pp} = -0.06666667$ $K_2^{pp} = 0.00533333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-99.40934426	-198.8190990	99.40975430	-1.99999588

	Orbital	1s	2s		2p
	Energy	-26.38270	-1.57251		-0.72999
ζ_1	6059261.1	.0000003	-.0000001		
ζ_2	1228911.8	.0000019	-.0000004		
ζ_3	286871.97	.0000109	-.0000025		
ζ_4	76276.739	.0000517	-.0000120		
ζ_5	22815.915	.0002135	-.0000494		
ζ_6	7570.7705	.0007747	-.0001795		
ζ_7	2745.2997	.0025308	-.0005871		
ζ_8	1071.4758	.0075480	-.0017601	ζ_8	.0000590
ζ_9	443.56400	.0208373	-.0049025	ζ_9	.0001512
ζ_{10}	192.17140	.0528959	-.0127316	ζ_{10}	.0007380
ζ_{11}	86.120725	.1208452	-.0303909	ζ_{11}	.0025899
ζ_{12}	39.536879	.2333337	-.0644713	ζ_{12}	.0088217
ζ_{13}	18.451801	.3403747	-.1147390	ζ_{13}	.0262771
ζ_{14}	8.7036210	.2835282	-.1421992	ζ_{14}	.0703151
ζ_{15}	4.1321847	.0847789	-.0354094	ζ_{15}	.1544392
ζ_{16}	1.9690336	.0051262	.2219039	ζ_{16}	.2527824
ζ_{17}	.94003492	.0013551	.4242460	ζ_{17}	.3028507
ζ_{18}	.44916062	.0001995	.3770787	ζ_{18}	.2692365
ζ_{19}	.21468142	.0001264	.1249543	ζ_{19}	.1486051
ζ_{20}	.10261793	-.0000069	.0064786	ζ_{20}	.0342894

Table 10. Ne ^{1}S (20s, 13p; 20 ζ)

		Symmetry species	S	P
		Number of basis functions	20	13
Nuclear charge	10	Number of closed shells	2	1
No. of electrons	10	Open-shell occupation	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-128.5470905	-257.0941840	128.5470930	-1.99999998

	Orbital	1s	2s		2p
	Energy	-32.77244	-1.93039		-0.85040
ζ_1	8133616.4	.0000003	-.0000001		
ζ_2	1642270.4	.0000017	-.0000004		
ζ_3	380773.80	.0000100	-.0000024		
ζ_4	100383.58	.0000483	-.0000113		
ζ_5	29737.527	.0002019	-.0000474		
ζ_6	9767.4661	.0007428	-.0001747		
ζ_7	3506.2154	.0024591	-.0005788		
ζ_8	1355.4374	.0074239	-.0017563	ζ_8	.0000587
ζ_9	556.27629	.0207155	-.0049456	ζ_9	.0001558
ζ_{10}	239.18204	.0530801	-.0129670	ζ_{10}	.0007613
ζ_{11}	106.49718	.1221874	-.0312288	ζ_{11}	.0027142
ζ_{12}	48.626798	.2369594	-.0667240	ζ_{12}	.0093458
ζ_{13}	22.591336	.3439614	-.1188174	ζ_{13}	.0281554
ζ_{14}	10.615476	.2800625	-.1436379	ζ_{14}	.0754163
ζ_{15}	5.0231969	.0799610	-.0253184	ζ_{15}	.1627671
ζ_{16}	2.3865241	.0048820	.2385824	ζ_{16}	.2588884
ζ_{17}	1.1362163	.0012963	.4299308	ζ_{17}	.3012268
ζ_{18}	.54146718	.0002743	.3638504	ζ_{18}	.2611261
ζ_{19}	.25813094	.0000950	.1133955	ζ_{19}	.1419457
ζ_{20}	.12306969	.0000019	.0054925	ζ_{20}	.0330683

Table 11. Na ^{2}S (23s, 13p; 23 ζ)

		Symmetry species	S	P
		Number of basis functions	23	13
Nuclear charge	11	Number of closed shells	2	1
No. of electrons	11	Open-shell occupation	1	0

Coupling coefficients
$K_0^{ss} = -1.00000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-161.8589015	-323.7178080	161.8589070	-1.99999996

	Orbital	1s	2s	3s		2p
	Energy	-40.47849	-2.79702	-0.18210		-1.51813
ζ_1	10841861.	.0000003	-.0000001	.0000000		
ζ_2	2193388.9	.0000015	-.0000004	.0000001		
ζ_3	509121.70	.0000089	-.0000022	.0000003		
ζ_4	134196.42	.0000428	-.0000104	.0000016		
ζ_5	39688.042	.0001795	-.0000438	.0000066		
ζ_6	12995.624	.0006640	-.0001623	.0000244		
ζ_7	4645.6061	.0022131	-.0005415	.0000814		
ζ_8	1787.4459	.0067319	-.0016555	.0002488	ζ_8	.0000555
ζ_9	730.19039	.0189332	-.0046943	.0007066	ζ_9	.0001501
ζ_{10}	312.74659	.0489526	-.0124108	.0018686	ζ_{10}	.0007357
ζ_{11}	138.89661	.1140425	-.0301707	.0045591	ζ_{11}	.0026505
ζ_{12}	63.367451	.2252404	-.0653967	.0099231	ζ_{12}	.0092209
ζ_{13}	29.472151	.3377123	-.1187410	.0182618	ζ_{13}	.0280884
ζ_{14}	13.891365	.2943664	-.1506573	.0236570	ζ_{14}	.0759540
ζ_{15}	6.6057465	.0963046	-.0444483	.0071831	ζ_{15}	.1659535
ζ_{16}	3.1589144	.0067008	.2215216	-.0389483	ζ_{16}	.2683096
ζ_{17}	1.5157244	.0016524	.4458970	-.0849459	ζ_{17}	.3155791
ζ_{18}	.72866576	.0000710	.3825848	-.1129255	ζ_{18}	.2605381
ζ_{19}	.35064238	.0002240	.1028136	-.1134832	ζ_{19}	.1100026
ζ_{20}	.16881043	-.0000969	.0020191	-.0133824	ζ_{20}	.0161711
ζ_{21}	.08128559	.0000546	.0006717	.3245628		
ζ_{22}	.03914291	-.0000252	-.0000301	.5733478		
ζ_{23}	.01884944	.0000060	.0001130	.2316942		

Table 12. Mg ^{1}S (23s, 13p; 23 ζ)

		Symmetry species	S	P
		Number of basis functions	23	13
Nuclear charge	12	Number of closed shells	3	1
No. of electrons	12	Open-shell occupation	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-199.6146236	-399.2292520	199.6146290	-1.99999997

	Orbital	1s	2s	3s		2p
	Energy	-49.03173	-3.76772	-0.25305		-2.28222
ζ_1	13213988.	.0000003	-.0000001	.0000000		
ζ_2	2744119.2	.0000014	-.0000004	.0000001		
ζ_3	645993.87	.0000082	-.0000021	.0000004		
ζ_4	170972.59	.0000394	-.0000099	.0000019		
ζ_5	50385.260	.0001669	-.0000422	.0000081		
ζ_6	16355.237	.0006269	-.0001586	.0000305		
ζ_7	5780.0158	.0021246	-.0005379	.0001037		
ζ_8	2197.3623	.0065664	-.0016707	.0003219	ζ_8	.0000565
ζ_9	887.98727	.0186994	-.0047974	.0009257	ζ_9	.0001589
ζ_{10}	377.16291	.0487611	-.0127932	.0024696	ζ_{10}	.0007787
ζ_{11}	166.63810	.1140085	-.0312399	.0060560	ζ_{11}	.0028357
ζ_{12}	75.890631	.2251817	-.0678110	.0132108	ζ_{12}	.0098770
ζ_{13}	35.352296	.3365098	-.1228903	.0243220	ζ_{13}	.0300722
ζ_{14}	16.738685	.2936282	-.1552541	.0314755	ζ_{14}	.0807852
ζ_{15}	8.0156338	.0981653	-.0465476	.0097778	ζ_{15}	.1745436
ζ_{16}	3.8674577	.0073018	.2259558	-.0518757	ζ_{16}	.2794233
ζ_{17}	1.8749364	.0015995	.4657422	-.1201456	ζ_{17}	.3239965
ζ_{18}	.91156004	.0000518	.3784539	-.1704700	ζ_{18}	.2455660
ζ_{19}	.44388387	.0001970	.0830086	-.1137445	ζ_{19}	.0816889
ζ_{20}	.21632024	-.0000915	.0019469	.1340380	ζ_{20}	.0103047
ζ_{21}	.10545696	.0000513	-.0002572	.4428272		
ζ_{22}	.05141703	-.0000227	.0001971	.4706414		
ζ_{23}	.02506989	.0000058	-.0000614	.1298506		

Table 13. Al ^{2}P (23s, 16p; 23 ζ)

		Symmetry species	S	P
		Number of basis functions	23	16
Nuclear charge	13	Number of closed shells	3	1
No. of electrons	13	Open-shell occupation	0	1

Coupling coefficients

$K_0^{pp} = -1.66666667$ $K_2^{pp} = 0.13333333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-241.8766931	-483.7533780	241.8766850	-2.00000003

	Orbital	1s	2s	3s		2p	3p
	Energy	-58.50101	-4.91066	-0.39341		-3.21829	-0.20995
ζ_1	17742122.	.0000002	-.0000001	.0000000			
ζ_2	3557452.1	.0000013	-.0000003	.0000001			
ζ_3	817621.36	.0000076	-.0000020	.0000005			
ζ_4	213296.12	.0000368	-.0000096	.0000022			
ζ_5	62436.936	.0001567	-.0000407	.0000094			
ζ_6	20246.910	.0005870	-.0001528	.0000353			
ζ_7	7174.6847	.0019780	-.0005150	.0001190			
ζ_8	2739.9513	.0060743	-.0015898	.0003671	ζ_8	.0000539	-.0000097
ζ_9	1112.5550	.0172315	-.0045431	.0010506	ζ_9	.0001496	-.0000268
ζ_{10}	474.34963	.0449770	-.0121196	.0028042	ζ_{10}	.0007317	-.0001320
ζ_{11}	210.00736	.1061735	-.0297940	.0069232	ζ_{11}	.0026789	-.0004815
ζ_{12}	95.630908	.2140614	-.0657589	.0153649	ζ_{12}	.0094292	-.0017072
ζ_{13}	44.442719	.3318428	-.1223020	.0290449	ζ_{13}	.0293253	-.0053245
ζ_{14}	20.949128	.3074643	-.1621411	.0395541	ζ_{14}	.0804973	-.0148516
ζ_{15}	9.9692277	.1120546	-.0612910	.0155576	ζ_{15}	.1787425	-.0334645
ζ_{16}	4.7731270	.0086637	.2242104	-.0623463	ζ_{16}	.2916318	-.0556172
ζ_{17}	2.2937812	.0018693	.4935196	-.1608440	ζ_{17}	.3385064	-.0670653
ζ_{18}	1.1046295	-.0001848	.3766293	-.2293812	ζ_{18}	.2321288	-.0523816
ζ_{19}	.53255201	.0003233	.0631299	-.0774376	ζ_{19}	.0609825	.0413111
ζ_{20}	.25688228	-.0001880	.0025372	.2997953	ζ_{20}	.0045288	.2157743
ζ_{21}	.12393628	.0001030	-.0010357	.5392195	ζ_{21}	.0006013	.3885855
ζ_{22}	.05979885	-.0000475	.0006843	.3244635	ζ_{22}	.0001817	.3622044
ζ_{23}	.02885320	.0000121	-.0001707	.0352610	ζ_{23}	.0000186	.1442626

Table 14. Si ^{3}P (23s, 16p; 23 ζ)

		Symmetry species	S	P
		Number of basis functions	23	16
Nuclear charge	14	Number of closed shells	3	1
No. of electrons	14	Open-shell occupation	0	2

Coupling coefficients

$K_0^{pp} = -0.66666667$ $K_2^{pp} = -0.06666667$

Total energy	Potential energy	Kinetic energy	Virial theorem
-288.8543479	-577.7086980	288.8543500	-1.99999999

	Orbital	1s	2s	3s		2p	3p
	Energy	-68.81244	-6.15652	-0.53983		-4.25604	-0.29711
ζ_1	23376525.	.0000002	-.0000001	.0000000			
ζ_2	4694045.0	.0000011	-.0000003	.0000001			
ζ_3	1076689.7	.0000065	-.0000017	.0000004			
ζ_4	279605.15	.0000318	-.0000085	.0000022			
ζ_5	81349.125	.0001365	-.0000363	.0000093			
ζ_6	26204.708	.0005160	-.0001375	.0000352			
ζ_7	9227.7394	.0017524	-.0004671	.0001197			
ζ_8	3505.9512	.0054159	-.0014507	.0003716	ζ_8	.0000477	-.0000102
ζ_9	1418.7245	.0154315	-.0041607	.0010675	ζ_9	.0001341	-.0000286
ζ_{10}	604.05175	.0404670	-.0111370	.0028587	ζ_{10}	.0006545	-.0001403
ζ_{11}	267.63283	.0962394	-.0274906	.0070879	ζ_{11}	.0024035	-.0005140
ζ_{12}	122.21563	.1973664	-.0613201	.0158942	ζ_{12}	.0084817	-.0018256
ζ_{13}	57.062831	.3177166	-.1164680	.0306827	ζ_{13}	.0265570	-.0057396
ζ_{14}	27.065543	.3216288	-.1643632	.0444651	ζ_{14}	.0736630	-.0161788
ζ_{15}	12.976149	.1396350	-.0896256	.0254104	ζ_{15}	.1678488	-.0375412
ζ_{16}	6.2650213	.0143254	.1796437	-.0556016	ζ_{16}	.2843309	-.0649504
ζ_{17}	3.0380195	.0022035	.4841117	-.1744006	ζ_{17}	.3435688	-.0817335
ζ_{18}	1.4769351	-.0003115	.4158650	-.2661515	ζ_{18}	.2432925	-.0626954
ζ_{19}	.71899652	.0004624	.0834901	-.0856275	ζ_{19}	.0657743	.0573270
ζ_{20}	.35025254	-.0002897	.0032186	.3270814	ζ_{20}	.0050809	.2590676
ζ_{21}	.17067018	.0001568	-.0005209	.5406577	ζ_{21}	.0006106	.4068245
ζ_{22}	.08317170	-.0000740	.0006214	.3124487	ζ_{22}	.0002276	.3246243
ζ_{23}	.04053251	.0000185	-.0001336	.0352809	ζ_{23}	.0000202	.1069525

Table 15. P ^{4}S (23s, 16p; 23 ζ)

		Symmetry species	S	P
		Number of basis functions	23	16
Nuclear charge	15	Number of closed shells	3	1
No. of electrons	15	Open-shell occupation	0	3

Coupling coefficients

$K_0^{pp} = -0.33333333$ $K_2^{pp} = -0.13333333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-340.7187652	-681.4375320	340.7187670	-1.99999999

	Orbital	1s	2s	3s		2p	3p
	Energy	-79.96970	-7.51108	-0.69641		-5.40095	-0.39170
ζ_1	28578316.	.0000002	.0000000	.0000000			
ζ_2	5799845.8	.0000010	-.0000003	.0000001			
ζ_3	1337455.4	.0000059	-.0000016	.0000004			
ζ_4	347673.61	.0000288	-.0000078	.0000022			
ζ_5	100925.88	.0001245	-.0000338	.0000093			
ζ_6	32369.229	.0004739	-.0001288	.0000354			
ζ_7	11337.532	.0016217	-.0004409	.0001212			
ζ_8	4284.5562	.0050486	-.0013792	.0003789	ζ_8	.0000446	-.0000106
ζ_9	1726.0005	.0144676	-.0039771	.0010942	ζ_9	.0001274	-.0000302
ζ_{10}	732.62856	.0381310	-.0106912	.0029434	ζ_{10}	.0006218	-.0001482
ζ_{11}	324.18302	.0911520	-.0264889	.0073242	ζ_{11}	.0022936	-.0005461
ζ_{12}	148.13044	.1886336	-.0594389	.0165287	ζ_{12}	.0081124	-.0019421
ζ_{13}	69.332080	.3092186	-.1140890	.0322404	ζ_{13}	.0254923	-.0061364
ζ_{14}	33.019677	.3270403	-.1657596	.0481488	ζ_{14}	.0710126	-.0173731
ζ_{15}	15.917404	.1554351	-.1042630	.0317763	ζ_{15}	.1635521	-.0408679
ζ_{16}	7.7354733	.0188683	.1555857	-.0517478	ζ_{16}	.2820335	-.0721454
ζ_{17}	3.7786579	.0022882	.4796678	-.1872133	ζ_{17}	.3467834	-.0927783
ζ_{18}	1.8515197	-.0003079	.4349223	-.2939948	ζ_{18}	.2456069	-.0678925
ζ_{19}	.90879143	.0004783	.0936872	-.0819698	ζ_{19}	.0653255	.0756206
ζ_{20}	.44645285	-.0003167	.0043180	.3502979	ζ_{20}	.0051089	.2912666
ζ_{21}	.21940782	.0001663	-.0002723	.5394481	ζ_{21}	.0003843	.4112288
ζ_{22}	.10784200	-.0000804	.0006754	.3002653	ζ_{22}	.0001753	.2941366
ζ_{23}	.05300772	.0000198	-.0001286	.0339507	ζ_{23}	-.0000229	.0855928

Table 16. S ^{3}P (23s, 16p; 23 ζ)

		Symmetry species	S	P
		Number of basis functions	23	16
Nuclear charge	16	Number of closed shells	3	1
No. of electrons	16	Open-shell occupation	0	4

Coupling coefficients

$K_0^{pp} = -0.16666667$ $K_2^{pp} = -0.01666667$

Total energy	Potential energy	Kinetic energy	Virial theorem
-397.5048764	-795.0097550	397.5048790	-1.99999999

	Orbital	1s	2s	3s		2p	3p
	Energy	-92.00444	-9.00428	-0.87952		-6.68250	-0.43736
ζ_1	32280958.	.0000002	.0000000	.0000000			
ζ_2	6606575.8	.0000010	-.0000003	.0000001			
ζ_3	1529008.4	.0000058	-.0000016	.0000005			
ζ_4	397307.34	.0000288	-.0000080	.0000023			
ζ_5	114926.04	.0001250	-.0000345	.0000100			
ζ_6	36648.695	.0004803	-.0001328	.0000386			
ζ_7	12747.324	.0016601	-.0004592	.0001333			
ζ_8	4782.2340	.0052171	-.0014499	.0004211	ζ_8	.0000478	-.0000122
ζ_9	1913.2413	.0150665	-.0042163	.0012251	ζ_9	.0001397	-.0000356
ζ_{10}	807.32289	.0398971	-.0113924	.0033175	ζ_{10}	.0006845	-.0001743
ζ_{11}	355.61730	.0954039	-.0283049	.0082682	ζ_{11}	.0025395	-.0006495
ζ_{12}	162.00913	.1961572	-.0633369	.0186552	ζ_{12}	.0090049	-.0023078
ζ_{13}	75.720053	.3158922	-.1205591	.0360597	ζ_{13}	.0282140	-.0073021
ζ_{14}	36.062847	.3215279	-.1701473	.0526479	ζ_{14}	.0780723	-.0205225
ζ_{15}	17.406573	.1431240	-.0950940	.0306050	ζ_{15}	.1762978	-.0475645
ζ_{16}	8.4785591	.0156512	.1845478	-.0649580	ζ_{16}	.2967654	-.0819736
ζ_{17}	4.1543358	.0020744	.5075406	-.2235289	ζ_{17}	.3486467	-.1026570
ζ_{18}	2.0429558	-.0003461	.4042688	-.3130768	ζ_{18}	.2199435	-.0552055
ζ_{19}	1.0067406	.0004177	.0688612	-.0119465	ζ_{19}	.0476310	.1286604
ζ_{20}	.49664328	-.0002943	.0052267	.4246593	ζ_{20}	.0039362	.3278991
ζ_{21}	.24512368	.0001479	-.0010335	.5250794	ζ_{21}	.0002893	.3885871
ζ_{22}	.12100584	-.0000728	.0010633	.2330683	ζ_{22}	.0004747	.2536989
ζ_{23}	.05973783	.0000177	-.0002221	.0194439	ζ_{23}	-.0000063	.0710414

Table 17. Cl ^{2}P (23s, 16p; 23 ζ)

		Symmetry species	S	P
		Number of basis functions	23	16
Nuclear charge	17	Number of closed shells	3	1
No. of electrons	17	Open-shell occupation	0	5

Coupling coefficients

$K_0^{pp} = -0.06666667$ $K_2^{pp} = 0.00533333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-459.4820498	-918.9641080	459.4820580	-1.99999998

	Orbital	1s	2s	3s		2p	3p
	Energy	-104.88441	-10.60747	-1.07290		-8.07221	-0.50639
ζ_1	36414299.	.0000002	.0000000	.0000000			
ζ_2	7544906.8	.0000010	-.0000003	.0000001			
ζ_3	1759266.2	.0000057	-.0000016	.0000005			
ζ_4	458649.48	.0000280	-.0000078	.0000024			
ζ_5	132659.61	.0001219	-.0000342	.0000103			
ζ_6	42194.517	.0004708	-.0001321	.0000400			
ζ_7	14614.816	.0016381	-.0004599	.0001391			
ζ_8	5455.7400	.0051842	-.0014619	.0004427	ζ_8	.0000484	-.0000130
ζ_9	2171.9126	.0150651	-.0042794	.0012956	ζ_9	.0001438	-.0000389
ζ_{10}	912.50775	.0400845	-.0116168	.0035276	ζ_{10}	.0007071	-.0001902
ζ_{11}	400.63161	.0961043	-.0289681	.0088181	ζ_{11}	.0026369	-.0007140
ζ_{12}	182.15531	.1976105	-.0648838	.0199459	ζ_{12}	.0093827	-.0025420
ζ_{13}	85.086192	.3170727	-.1234382	.0385152	ζ_{13}	.0294024	-.0080637
ζ_{14}	40.554625	.3202448	-.1729294	.0560372	ζ_{14}	.0812288	-.0226247
ζ_{15}	19.613333	.1411866	-.0943801	.0316507	ζ_{15}	.1820427	-.0522046
ζ_{16}	9.5820439	.0152773	.1943687	-.0715050	ζ_{16}	.3040853	-.0894331
ζ_{17}	4.7128247	.0019771	.5202664	-.2485511	ζ_{17}	.3488520	-.1103073
ζ_{18}	2.3277462	-.0003673	.3911041	-.3237515	ζ_{18}	.2060259	-.0444498
ζ_{19}	1.1525590	.0003886	.0606666	.0304451	ζ_{19}	.0401698	.1615936
ζ_{20}	.57143297	-.0002907	.0059529	.4578961	ζ_{20}	.0037337	.3443864
ζ_{21}	.28349078	.0001408	-.0012032	.5094666	ζ_{21}	.0004060	.3736084
ζ_{22}	.14067574	-.0000705	.0011994	.2033756	ζ_{22}	.0006546	.2299057
ζ_{23}	.06981206	.0000170	-.0002480	.0153100	ζ_{23}	.0000212	.0624540

Table 18. Ar ^{1}S (23s, 16p; 23 ζ)

		Symmetry species	S	P
		Number of basis functions	23	16
Nuclear charge	18	Number of closed shells	3	2
No. of electrons	18	Open-shell occupation	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-526.8174873	-1053.634990	526.8175060	-1.99999996

	Orbital	1s	2s	3s		2p	3p
	Energy	-118.61033	-12.32214	-1.27734		-9.57145	-0.59101
ζ_1	42167954.	.0000002	.0000000	.0000000			
ζ_2	8762963.1	.0000009	-.0000003	.0000001			
ζ_3	2044974.7	.0000054	-.0000015	.0000005			
ζ_4	532637.44	.0000269	-.0000076	.0000024			
ζ_5	153710.24	.0001174	-.0000333	.0000104			
ζ_6	48735.891	.0004556	-.0001295	.0000405			
ζ_7	16820.084	.0015930	-.0004531	.0001415			
ζ_8	6256.4667	.0050655	-.0014466	.0004526	ζ_8	.0000478	-.0000133
ζ_9	2482.6632	.0147801	-.0042523	.0013296	ζ_9	.0001435	-.0000403
ζ_{10}	1040.3915	.0394598	-.0115786	.0036331	ζ_{10}	.0007074	-.0001972
ζ_{11}	455.99427	.0948756	-.0289577	.0091048	ζ_{11}	.0026465	-.0007436
ζ_{12}	207.16764	.1956954	-.0650283	.0206659	ζ_{12}	.0094451	-.0026535
ζ_{13}	96.788131	.3153648	-.1241727	.0400397	ζ_{13}	.0296496	-.0084433
ζ_{14}	46.182585	.3215505	-.1749533	.0587161	ζ_{14}	.0820549	-.0237391
ζ_{15}	22.377399	.1446815	-.0985827	.0341972	ζ_{15}	.1839545	-.0549191
ζ_{16}	10.960336	.0162236	.1934373	-.0736412	ζ_{16}	.3078635	-.0944951
ζ_{17}	5.4072874	.0019515	.5267559	-.2659692	ζ_{17}	.3498841	-.1158174
ζ_{18}	2.6799809	-.0003952	.3887616	-.3327506	ζ_{18}	.1992779	-.0365288
ζ_{19}	1.3318957	.0003825	.0589887	.0547498	ζ_{19}	.0364699	.1828833
ζ_{20}	.66290901	-.0003022	.0065537	.4742553	ζ_{20}	.0029852	.3539844
ζ_{21}	.33017812	.0001424	-.0011839	.4995673	ζ_{21}	-.0002425	.3638557
ζ_{22}	.16450060	-.0000724	.0012619	.1893692	ζ_{22}	.0002974	.2141661
ζ_{23}	.08196417	.0000173	-.0002554	.0137910	ζ_{23}	-.0000804	.0563511

Table 19. K ^{2}S (26s, 16p; 26 ζ)

		Symmetry species	S	P
		Number of basis functions	26	16
Nuclear charge	19	Number of closed shells	3	2
No. of electrons	19	Open-shell occupation	1	0

Coupling coefficients
$K_0^{ss} = -1.00000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-599.1647582	-1198.329540	599.1647770	-1.99999998

	Orbital	1s	2s	3s	4s
	Energy	-133.53303	-14.48994	-1.74877	-0.14747
ζ_1	45541929.	.0000002	.0000000	.0000000	.0000000
ζ_2	9727872.5	.0000009	-.0000003	.0000001	.0000000
ζ_3	2319268.4	.0000053	-.0000015	.0000005	-.0000001
ζ_4	613552.70	.0000255	-.0000073	.0000024	-.0000005
ζ_5	178871.62	.0001106	-.0000318	.0000105	-.0000020
ζ_6	57024.964	.0004277	-.0001230	.0000405	-.0000078
ζ_7	19713.536	.0014972	-.0004308	.0001419	-.0000274
ζ_8	7324.4672	.0047809	-.0013809	.0004556	-.0000880
ζ_9	2898.3116	.0140307	-.0040820	.0013458	-.0002599
ζ_{10}	1210.4578	.0377089	-.0111814	.0036998	-.0007146
ζ_{11}	528.95507	.0912959	-.0281298	.0093259	-.0018023
ζ_{12}	239.90274	.1898911	-.0635537	.0213017	-.0041194
ζ_{13}	112.10231	.3098964	-.1222946	.0415854	-.0080592
ζ_{14}	53.623621	.3248733	-.1755175	.0621507	-.0120850
ζ_{15}	26.113543	.1552967	-.1091722	.0400581	-.0078411
ζ_{16}	12.887057	.0197310	.1716682	-.0687422	.0135762
ζ_{17}	6.4211480	.0020194	.5150987	-.2735047	.0557295
ζ_{18}	3.2209352	-.0004009	.4089950	-.3573838	.0768042
ζ_{19}	1.6229457	.0004299	.0728207	.0276850	-.0108046
ζ_{20}	.82011791	-.0003817	.0078280	.4890199	-.1199762
ζ_{21}	.41514963	.0002296	-.0018058	.5310021	-.1682543
ζ_{22}	.21035757	-.0001687	.0023305	.1736066	-.1708659
ζ_{23}	.10664212	.0001053	-.0014088	.0063678	-.0586831
ζ_{24}	.05407500	-.0000593	.0008205	.0014231	.3452510
ζ_{25}	.02742205	.0000260	-.0003690	-.0001862	.6062155
ζ_{26}	.01390634	-.0000064	.0000905	.0002339	.2372364

Table 19. K ^{2}S (26s, 16p; 26 ζ) (continued)

	Orbital	2p	3p
	Energy	-11.51926	-0.95441
ζ_8	7324.4672	.0000449	-.0000136
ζ_9	2898.3116	.0001363	-.0000417
ζ_{10}	1210.4578	.0006743	-.0002052
ζ_{11}	528.95507	.0025418	-.0007790
ζ_{12}	239.90274	.0091131	-.0027949
ζ_{13}	112.10231	.0287040	-.0089205
ζ_{14}	53.623621	.0795638	-.0251455
ζ_{15}	26.113543	.1791312	-.0584700
ζ_{16}	12.887057	.3025804	-.1018061
ζ_{17}	6.4211480	.3493395	-.1265370
ζ_{18}	3.2209352	.2060203	-.0431086
ζ_{19}	1.6229457	.0412208	.1899722
ζ_{20}	.82011791	.0033029	.3754707
ζ_{21}	.41514963	-.0001973	.3792129
ζ_{22}	.21035757	.0002606	.1800039
ζ_{23}	.10664212	-.0000842	.0340695

Table 20. Ca ^{1}S (26s, 16p; 26 ζ)

		Symmetry species	S	P
		Number of basis functions	26	16
Nuclear charge	20	Number of closed shells	4	2
No. of electrons	20	Open-shell occupation	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-676.7581540	-1353.516340	676.7581850	-1.99999996

	Orbital	1s	2s	3s	4s
	Energy	-149.36371	-16.82273	-2.24537	-0.19552
ζ_1	53505253.	.0000002	.0000000	.0000000	.0000000
ζ_2	11371432.	.0000009	-.0000002	.0000001	.0000000
ζ_3	2699633.4	.0000050	-.0000014	.0000005	-.0000001
ζ_4	711711.53	.0000242	-.0000070	.0000024	-.0000006
ζ_5	206930.71	.0001051	-.0000305	.0000105	-.0000025
ζ_6	65841.122	.0004073	-.0001183	.0000408	-.0000097
ζ_7	22732.138	.0014273	-.0004150	.0001430	-.0000342
ζ_8	8440.3762	.0045609	-.0013311	.0004597	-.0001097
ζ_9	3339.4469	.0133899	-.0039349	.0013574	-.0003242
ζ_{10}	1395.1510	.0360244	-.0107843	.0037351	-.0008920
ζ_{11}	610.09171	.0874667	-.0271733	.0094255	-.0022529
ζ_{12}	276.97780	.1832426	-.0616838	.0216428	-.0051761
ζ_{13}	129.58522	.3036213	-.1198180	.0426198	-.0102208
ζ_{14}	62.072525	.3287646	-.1759977	.0652536	-.0157040
ζ_{15}	30.273376	.1668183	-.1196265	.0459786	-.0111623
ζ_{16}	14.963495	.0234131	.1542140	-.0643292	.0157777
ζ_{17}	7.4678575	.0020845	.5118595	-.2856003	.0725465
ζ_{18}	3.7521526	-.0003975	.4232978	-.3816002	.1030316
ζ_{19}	1.8937514	.0004351	.0797448	.0231032	-.0129423
ζ_{20}	.95855642	-.0003998	.0081790	.5347590	-.1661328
ζ_{21}	.48603616	.0002412	-.0017632	.5419288	-.2635157
ζ_{22}	.24668572	-.0001764	.0022396	.1315214	-.1880693
ζ_{23}	.12526678	.0001108	-.0013917	.0044355	.1400082
ζ_{24}	.06362451	-.0000624	.0008103	-.0004503	.5035907
ζ_{25}	.03231828	.0000273	-.0003609	.0003170	.4826979
ζ_{26}	.01641654	-.0000068	.0000903	-.0000944	.1022744

Table 20. Ca ^{1}S (26s, 16p; 26 ζ) (continued)

	Orbital	2p	3p
	Energy	-13.62925	-1.34070
ζ_8	8440.3762	.0000428	-.0000139
ζ_9	3339.4469	.0001300	-.0000425
ζ_{10}	1395.1510	.0006431	-.0002089
ζ_{11}	610.09171	.0024243	-.0007946
ζ_{12}	276.97780	.0087093	-.0028534
ζ_{13}	129.58522	.0275442	-.0091547
ζ_{14}	62.072525	.0768662	-.0259682
ζ_{15}	30.273376	.1751157	-.0612197
ζ_{16}	14.963495	.3005389	-.1084390
ζ_{17}	7.4678575	.3521827	-.1369842
ζ_{18}	3.7521526	.2100435	-.0452640
ζ_{19}	1.8937514	.0425134	.2072197
ζ_{20}	.95855642	.0032670	.4074475
ζ_{21}	.48603616	-.0002427	.3779959
ζ_{22}	.24668572	.0002386	.1373083
ζ_{23}	.12526678	-.0000971	.0216011

Table 21. Sc ^{2}D (26s, 17p, 13d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	17	13
Nuclear charge	21	Number of closed shells	4	2	0
No. of electrons	21	Open-shell occupation	0	0	1

Coupling coefficients

$K_0^{dd} = -1.80000000$ $K_2^{dd} = 0.05714286$ $K_4^{dd} = 0.05714286$

Total energy	Potential energy	Kinetic energy	Virial theorem
-759.7356986	-1519.471440	759.7357380	-1.99999995

	Orbital	1s	2s	3s	4s
	Energy	-165.89988	-19.08060	-2.56731	-0.21010
ζ_1	27624024.	.0000004	-.0000001	.0000000	.0000000
ζ_2	5892699.9	.0000022	-.0000006	.0000002	-.0000001
ζ_3	1424192.1	.0000123	-.0000036	.0000013	-.0000003
ζ_4	386819.17	.0000570	-.0000167	.0000059	-.0000014
ζ_5	116960.97	.0002336	-.0000685	.0000241	-.0000057
ζ_6	38960.314	.0008474	-.0002485	.0000876	-.0000208
ζ_7	14138.214	.0027674	-.0008139	.0002866	-.0000680
ζ_8	5525.3488	.0082216	-.0024289	.0008571	-.0002034
ζ_9	2299.1501	.0223915	-.0066999	.0023628	-.0005607
ζ_{10}	1007.6090	.0556170	-.0170617	.0060472	-.0014359
ζ_{11}	460.45047	.1232370	-.0399257	.0141953	-.0033718
ζ_{12}	217.45536	.2304715	-.0829470	.0299406	-.0071255
ζ_{13}	105.32321	.3254587	-.1446774	.0532590	-.0127062
ζ_{14}	51.984008	.2754417	-.1723702	.0667921	-.0160381
ζ_{15}	26.011445	.0969356	-.0469397	.0183653	-.0044226
ζ_{16}	13.141658	.0082604	.2869937	-.1321471	.0324371
ζ_{17}	6.6832952	.0011344	.5444370	-.3649626	.0945356
ζ_{18}	3.4135234	-.0001964	.2958970	-.3028153	.0812880
ζ_{19}	1.7481912	.0001140	.0344208	.2126107	-.0675909
ζ_{20}	.89675308	-.0001463	.0051311	.6062127	-.2036458
ζ_{21}	.46041065	.0000686	-.0011016	.4175184	-.2594348
ζ_{22}	.23649218	-.0000524	.0013007	.0587786	-.1049342
ζ_{23}	.12150088	.0000322	-.0007833	.0051228	.2276319
ζ_{24}	.06242778	-.0000179	.0004464	-.0023455	.5229091
ζ_{25}	.03207654	.0000078	-.0001954	.0011238	.4049450
ζ_{26}	.01648161	-.0000019	.0000481	-.0002883	.0667093

Table 21. Sc ^{2}D (26s, 17p, 13d; 26 ζ) (continued)

	Orbital	2p	3p		3d
	Energy	-15.66823	-1.57453		-0.34371
ζ_7	14138.214	.0000210	-.0000071		
ζ_8	5525.3488	.0000667	-.0000224		
ζ_9	2299.1501	.0003255	-.0001095		
ζ_{10}	1007.6090	.0012400	-.0004168		
ζ_{11}	460.45047	.0044679	-.0015099		
ζ_{12}	217.45536	.0145403	-.0049397	ζ_{12}	.0001784
ζ_{13}	105.32321	.0423467	-.0146061	ζ_{13}	.0004588
ζ_{14}	51.984008	.1075971	-.0380189	ζ_{14}	.0022825
ζ_{15}	26.011445	.2179273	-.0796465	ζ_{15}	.0076840
ζ_{16}	13.141658	.3303835	-.1262917	ζ_{16}	.0224517
ζ_{17}	6.6832952	.3186265	-.1271259	ζ_{17}	.0555669
ζ_{18}	3.4135234	.1397084	.0324214	ζ_{18}	.1224097
ζ_{19}	1.7481912	.0194435	.2945635	ζ_{19}	.2044871
ζ_{20}	.89675308	.0014057	.4243408	ζ_{20}	.2662323
ζ_{21}	.46041065	-.0000269	.3020398	ζ_{21}	.2786191
ζ_{22}	.23649218	.0000976	.0792859	ζ_{22}	.2309605
ζ_{23}	.12150088	-.0000367	.0112366	ζ_{23}	.1256429
ζ_{24}	.06242778			ζ_{24}	.0482124

Table 22. Ti ^{3}F (26s, 17p, 13d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	17	13
Nuclear charge	22	Number of closed shells	4	2	0
No. of electrons	22	Open-shell occupation	0	0	2

Coupling coefficients

$K_0^{dd} = -0.80000000$ $K_2^{dd} = -0.10612245$ $K_4^{dd} = 0.03673469$

Total energy	Potential energy	Kinetic energy	Virial theorem
-848.4059758	-1696.812030	848.4060500	-1.99999992

	Orbital	1s	2s	3s	4s
	Energy	-183.27274	-21.42289	-2.87338	-0.22078
ζ_1	31974270.	.0000004	-.0000001	.0000000	.0000000
ζ_2	6845386.9	.0000020	-.0000006	.0000002	.0000000
ζ_3	1658413.9	.0000114	-.0000034	.0000012	-.0000003
ζ_4	451045.71	.0000528	-.0000156	.0000056	-.0000013
ζ_5	136451.16	.0002166	-.0000640	.0000229	-.0000053
ζ_6	45447.752	.0007863	-.0002326	.0000832	-.0000193
ζ_7	16484.028	.0025711	-.0007623	.0002724	-.0000633
ζ_8	6437.5646	.0076520	-.0022788	.0008160	-.0001896
ζ_9	2676.7878	.0208949	-.0062976	.0022535	-.0005235
ζ_{10}	1172.4007	.0521258	-.0160901	.0057867	-.0013451
ζ_{11}	535.54983	.1164232	-.0378468	.0136505	-.0031744
ζ_{12}	252.89520	.2209234	-.0794056	.0290697	-.0067721
ζ_{13}	122.51178	.3208024	-.1409425	.0525790	-.0122798
ζ_{14}	60.496948	.2862702	-.1756241	.0689136	-.0161945
ζ_{15}	30.293754	.1103056	-.0652432	.0262496	-.0062014
ζ_{16}	15.320112	.0105801	.2613913	-.1213411	.0291448
ζ_{17}	7.8001886	.0012962	.5453278	-.3635413	.0919444
ζ_{18}	3.9891568	-.0002820	.3204510	-.3244344	.0854155
ζ_{19}	2.0458573	.0001955	.0414478	.1906421	-.0600548
ζ_{20}	1.0509883	-.0002095	.0057453	.5996322	-.1957992
ζ_{21}	.54041627	.0001128	-.0012557	.4342424	-.2491465
ζ_{22}	.27801570	-.0000832	.0014990	.0705747	-.1157908
ζ_{23}	.14305645	.0000517	-.0009063	.0049942	.1888628
ζ_{24}	.07361802	-.0000289	.0005191	-.0019426	.4888687
ζ_{25}	.03788550	.0000125	-.0002275	.0009574	.4382386
ζ_{26}	.01949686	-.0000031	.0000560	-.0002477	.1012599

Table 22. Ti ^{3}F (26s, 17p, 13d; 26 ζ) (continued)

	Orbital	2p	3p		3d
	Energy	-17.79117	-1.79507		-0.44065
ζ_7	16484.028	.0000192	-.0000066		
ζ_8	6437.5646	.0000612	-.0000210		
ζ_9	2676.7878	.0002991	-.0001028		
ζ_{10}	1172.4007	.0011424	-.0003922		
ζ_{11}	535.54983	.0041309	-.0014262		
ζ_{12}	252.89520	.0135215	-.0046910	ζ_{12}	.0001833
ζ_{13}	122.51178	.0396913	-.0139807	ζ_{13}	.0004754
ζ_{14}	60.496948	.1021081	-.0368325	ζ_{14}	.0023707
ζ_{15}	30.293754	.2108591	-.0787628	ζ_{15}	.0081016
ζ_{16}	15.320112	.3270429	-.1277467	ζ_{16}	.0240371
ζ_{17}	7.8001886	.3250643	-.1326937	ζ_{17}	.0601372
ζ_{18}	3.9891568	.1489224	.0246564	ζ_{18}	.1319127
ζ_{19}	2.0458573	.0220047	.2912106	ζ_{19}	.2182300
ζ_{20}	1.0509883	.0017051	.4232323	ζ_{20}	.2772812
ζ_{21}	.54041627	.0000082	.3062653	ζ_{21}	.2788268
ζ_{22}	.27801570	.0001379	.0844582	ζ_{22}	.2137935
ζ_{23}	.14305645	-.0000375	.0120421	ζ_{23}	.1057983
ζ_{24}	.07361802			ζ_{24}	.0333607

Table 23. V ^{4}F (26s, 17p, 13d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	17	13
Nuclear charge	23	Number of closed shells	4	2	0
No. of electrons	23	Open-shell occupation	0	0	3

Coupling coefficients

$K_0^{dd} = -0.46666667$ $K_2^{dd} = -0.07891156$ $K_4^{dd} = -0.01541950$

Total energy	Potential energy	Kinetic energy	Virial theorem
-942.8843137	-1885.768780	942.8844680	-1.99999983

	Orbital	1s	2s	3s	4s
	Energy	-201.50280	-23.87463	-3.18317	-0.23057
ζ_1	36641923.	.0000004	-.0000001	.0000000	.0000000
ζ_2	7842176.5	.0000019	-.0000006	.0000002	.0000000
ζ_3	1899441.1	.0000107	-.0000032	.0000012	-.0000003
ζ_4	516500.12	.0000499	-.0000149	.0000054	-.0000012
ζ_5	156226.83	.0002046	-.0000609	.0000220	-.0000050
ζ_6	52025.923	.0007429	-.0002214	.0000801	-.0000182
ζ_7	18866.442	.0024304	-.0007259	.0002624	-.0000596
ζ_8	7366.2961	.0072399	-.0021718	.0007867	-.0001787
ζ_9	3062.0876	.0198039	-.0060090	.0021749	-.0004941
ζ_{10}	1340.6858	.0495693	-.0153915	.0055990	-.0012727
ζ_{11}	612.16380	.1114207	-.0363643	.0132642	-.0030164
ζ_{12}	288.93170	.2138811	-.0769179	.0284735	-.0064862
ζ_{13}	139.89155	.3171510	-.1384285	.0521934	-.0119202
ζ_{14}	69.036953	.2939272	-.1780040	.0705621	-.0162119
ζ_{15}	34.547373	.1204133	-.0777672	.0318349	-.0073619
ζ_{16}	17.459062	.0124995	.2458432	-.1152766	.0270795
ζ_{17}	8.8827648	.0013940	.5470264	-.3657604	.0903301
ζ_{18}	4.5394020	-.0003423	.3345056	-.3363434	.0866183
ζ_{19}	2.3262725	.0002513	.0453796	.1846769	-.0571671
ζ_{20}	1.1941154	-.0002523	.0061129	.5979872	-.1907472
ζ_{21}	.61353198	.0001438	-.0013471	.4383900	-.2398185
ζ_{22}	.31538196	-.0001044	.0016069	.0753735	-.1170051
ζ_{23}	.16215594	.0000653	-.0009731	.0049138	.1665572
ζ_{24}	.08338099	-.0000365	.0005588	-.0017198	.4657782
ζ_{25}	.04287591	.0000158	-.0002452	.0008645	.4505704
ζ_{26}	.02204765	-.0000039	.0000604	-.0002250	.1279517

Table 23. V ^{4}F (26s, 17p, 13d; 26 ζ) (continued)

	Orbital	2p	3p		3d
	Energy	-20.02247	-2.01921		-0.50961
ζ_7	18866.442	.0000180	-.0000063		
ζ_8	7366.2961	.0000575	-.0000200		
ζ_9	3062.0876	.0002807	-.0000982		
ζ_{10}	1340.6858	.0010745	-.0003752		
ζ_{11}	612.16380	.0038974	-.0013687		
ζ_{12}	288.93170	.0128290	-.0045261	ζ_{12}	.0001857
ζ_{13}	139.89155	.0379404	-.0135901	ζ_{13}	.0004870
ζ_{14}	69.036953	.0986662	-.0361913	ζ_{14}	.0024354
ζ_{15}	34.547373	.2068857	-.0786578	ζ_{15}	.0084361
ζ_{16}	17.459062	.3261357	-.1297564	ζ_{16}	.0253731
ζ_{17}	8.8827648	.3292243	-.1365631	ζ_{17}	.0641186
ζ_{18}	4.5394020	.1533018	.0231553	ζ_{18}	.1398436
ζ_{19}	2.3262725	.0230799	.2939391	ζ_{19}	.2279551
ζ_{20}	1.1941154	.0018890	.4233862	ζ_{20}	.2826584
ζ_{21}	.61353198	.0000437	.3045940	ζ_{21}	.2750813
ζ_{22}	.31538196	.0001654	.0848823	ζ_{22}	.2021481
ζ_{23}	.16215594	-.0000358	.0119324	ζ_{23}	.0954780
ζ_{24}	.08338099			ζ_{24}	.0279455

Table 24. Cr ^{7}S (26s, 17p, 13d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	17	13
Nuclear charge	24	Number of closed shells	3	2	0
No. of electrons	24	Open-shell occupation	1	0	5

Coupling coefficients

$K_0^{ss} = -1.00000000$
$K_0^{dd} = -0.20000000 \quad K_2^{dd} = -0.05714286 \quad K_4^{dd} = -0.05714286$
$K_2^{sd} = -0.20000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-1043.356337	-2086.712020	1043.355680	-2.00000063

	Orbital	1s	2s	3s	4s
	Energy	-220.38641	-26.20963	-3.28514	-0.22203
ζ_1	39452193.	.0000004	-.0000001	.0000000	.0000000
ζ_2	8183165.5	.0000021	-.0000006	.0000002	.0000000
ζ_3	1941276.7	.0000118	-.0000035	.0000013	-.0000003
ζ_4	521633.59	.0000552	-.0000166	.0000060	-.0000013
ζ_5	157005.15	.0002267	-.0000680	.0000246	-.0000052
ζ_6	52286.928	.0008202	-.0002460	.0000891	-.0000188
ζ_7	19017.873	.0026665	-.0008024	.0002904	-.0000613
ζ_8	7456.0343	.0078904	-.0023836	.0008642	-.0001826
ζ_9	3110.8782	.0214675	-.0065710	.0023818	-.0005033
ζ_{10}	1364.9391	.0535035	-.0167697	.0061074	-.0012916
ζ_{11}	623.09991	.1197204	-.0396343	.0144907	-.0030649
ζ_{12}	293.22729	.2274571	-.0834998	.0309898	-.0065694
ζ_{13}	141.15770	.3278167	-.1487254	.0564272	-.0119889
ζ_{14}	69.080328	.2821275	-.1800721	.0719694	-.0154024
ζ_{15}	34.201064	.0983457	-.0460683	.0190631	-.0040867
ζ_{16}	17.067060	.0073478	.3270577	-.1622868	.0356172
ζ_{17}	8.5612492	.0011012	.5632804	-.4142744	.0961811
ζ_{18}	4.3086647	-.0003291	.2526572	-.2473400	.0591775
ζ_{19}	2.1727396	.0001745	.0219802	.3411934	-.0961209
ζ_{20}	1.0968856	-.0001780	.0039921	.6080822	-.1980766
ζ_{21}	.55408178	.0000986	-.0006946	.3248951	-.1914591
ζ_{22}	.27997009	-.0000696	.0008112	.0364859	-.0600857
ζ_{23}	.14148265	.0000434	-.0004252	.0042225	.1977543
ζ_{24}	.07150136	-.0000242	.0003551	-.0019402	.4948122
ζ_{25}	.03613524	.0000107	-.0000371	.0007504	.4120815
ζ_{26}	.01826201	-.0000026	.0000425	-.0002479	.0745223

Table 24. Cr ^{7}S (26s, 17p, 13d; 26 ζ) (continued)

	Orbital	2p	3p		3d
	Energy	-22.13986	-2.05091		-0.37359
ζ_7	19017.873	.0000209	-.0000073		
ζ_8	7456.0343	.0000658	-.0000230		
ζ_9	3110.8782	.0003200	-.0001119		
ζ_{10}	1364.9391	.0012224	-.0004289		
ζ_{11}	623.09991	.0044344	-.0015596		
ζ_{12}	293.22729	.0146694	-.0052031	ζ_{12}	.0002163
ζ_{13}	141.15770	.0435723	-.0156743	ζ_{13}	.0005869
ζ_{14}	69.080328	.1131299	-.0418782	ζ_{14}	.0029287
ζ_{15}	34.201064	.2325433	-.0892326	ζ_{15}	.0102266
ζ_{16}	17.067060	.3497561	-.1419055	ζ_{16}	.0305665
ζ_{17}	8.5612492	.3097799	-.1219133	ζ_{17}	.0772399
ζ_{18}	4.3086647	.1117342	.0925363	ζ_{18}	.1599351
ζ_{19}	2.1727396	.0119108	.3571905	ζ_{19}	.2398096
ζ_{20}	1.0968856	.0011025	.4127993	ζ_{20}	.2747616
ζ_{21}	.55408178	.0002087	.2410984	ζ_{21}	.2535387
ζ_{22}	.27997009	.0000750	.0544761	ζ_{22}	.1958341
ζ_{23}	.14148265	.0000125	.0064314	ζ_{23}	.1067901
ζ_{24}	.07150136			ζ_{24}	.0416397

Table 25. Mn ^{6}S (26s, 17p, 13d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	17	13
Nuclear charge	25	Number of closed shells	4	2	0
No. of electrons	25	Open-shell occupation	0	0	5

Coupling coefficients

$K_0^{dd} = -0.20000000$ $K_2^{dd} = -0.05714286$ $K_4^{dd} = -0.05714286$

Total energy	Potential energy	Kinetic energy	Virial theorem
-1149.866220	-2299.732920	1149.866700	-1.99999958

	Orbital	1s	2s	3s	4s
	Energy	-240.53394	-29.10943	-3.81661	-0.24786
ζ_1	47145111.	.0000003	-.0000001	.0000000	.0000000
ζ_2	10045644.	.0000017	-.0000005	.0000002	.0000000
ζ_3	2426015.7	.0000098	-.0000029	.0000011	-.0000002
ζ_4	658562.00	.0000455	-.0000137	.0000050	-.0000011
ζ_5	199043.01	.0001865	-.0000563	.0000207	-.0000045
ζ_6	66275.244	.0006772	-.0002044	.0000752	-.0000163
ζ_7	24038.518	.0022153	-.0006701	.0002462	-.0000534
ζ_8	9388.1747	.0066029	-.0020055	.0007385	-.0001601
ζ_9	3902.9530	.0181000	-.0055564	.0020442	-.0004433
ζ_{10}	1708.4470	.0455417	-.0142874	.0052833	-.0011460
ζ_{11}	779.55716	.1034533	-.0340117	.0126071	-.0027364
ζ_{12}	367.50658	.2024530	-.0729496	.0274373	-.0059638
ζ_{13}	177.63671	.3105992	-.1343703	.0514353	-.0112114
ζ_{14}	87.476138	.3055557	-.1814297	.0729670	-.0159908
ζ_{15}	43.662583	.1373670	-.0969967	.0405953	-.0089720
ζ_{16}	22.001430	.0160806	.2233036	-.1064619	.0238871
ζ_{17}	11.158190	.0015203	.5508290	-.3711267	.0872425
ζ_{18}	5.6828864	-.0004246	.3536185	-.3515409	.0863683
ζ_{19}	2.9019530	.0003298	.0502911	.1828543	-.0542421
ζ_{20}	1.4841962	-.0003114	.0066302	.5972807	-.1813662
ζ_{21}	.75974773	.0001879	-.0014988	.4392916	-.2232207
ζ_{22}	.38908091	-.0001343	.0017593	.0796423	-.1140343
ζ_{23}	.19929586	.0000844	-.0010686	.0047430	.1341898
ζ_{24}	.10209183	-.0000473	.0006155	-.0014527	.4325075
ζ_{25}	.05229912	.0000206	-.0002709	.0007520	.4566469
ζ_{26}	.02679169	-.0000051	.0000670	-.0001979	.1749375

Table 25. Mn ^{6}S (26s, 17p, 13d; 26 ζ) (continued)

	Orbital	2p	3p		3d
	Energy	-24.81254	-2.47950		-0.63882
ζ_7	24038.518	.0000162	-.0000058		
ζ_8	9388.1747	.0000517	-.0000184		
ζ_9	3902.9530	.0002527	-.0000906		
ζ_{10}	1708.4470	.0009703	-.0003473		
ζ_{11}	779.55716	.0035379	-.0012741		
ζ_{12}	367.50658	.0117666	-.0042555	ζ_{12}	.0001862
ζ_{13}	177.63671	.0352844	-.0129562	ζ_{13}	.0004994
ζ_{14}	87.476138	.0935730	-.0351823	ζ_{14}	.0025122
ζ_{15}	43.662583	.2014242	-.0786247	ζ_{15}	.0089235
ζ_{16}	22.001430	.3260640	-.1334106	ζ_{16}	.0275103
ζ_{17}	11.158190	.3357427	-.1423927	ζ_{17}	.0707927
ζ_{18}	5.6828864	.1583537	.0240847	ζ_{18}	.1528829
ζ_{19}	2.9019530	.0240318	.3017896	ζ_{19}	.2426006
ζ_{20}	1.4841962	.0021530	.4239948	ζ_{20}	.2887765
ζ_{21}	.75974773	.0000998	.2989859	ζ_{21}	.2672857
ζ_{22}	.38908091	.0002070	.0832633	ζ_{22}	.1851853
ζ_{23}	.19929586	-.0000333	.0111781	ζ_{23}	.0820068
ζ_{24}	.10209183			ζ_{24}	.0216463

Table 26. Fe ^{5}D (26s, 17p, 13d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	17	13
Nuclear charge	26	Number of closed shells	4	2	0
No. of electrons	26	Open-shell occupation	0	0	6

Coupling coefficients

$K_0^{dd} = -0.13333333 \quad K_2^{dd} = -0.02222222 \quad K_4^{dd} = -0.02222222$

Total energy	Potential energy	Kinetic energy	Virial theorem
-1262.443628	-2524.887830	1262.444200	-1.99999955

	Orbital	1s	2s	3s	4s
	Energy	-261.37336	-31.93547	-4.16940	-0.25817
ζ_1	53946029.	.0000003	-.0000001	.0000000	.0000000
ζ_2	11304393.	.0000017	-.0000005	.0000002	.0000000
ζ_3	2697672.1	.0000095	-.0000029	.0000011	-.0000002
ζ_4	726658.11	.0000446	-.0000135	.0000050	-.0000011
ζ_5	218683.93	.0001835	-.0000557	.0000206	-.0000044
ζ_6	72696.529	.0006663	-.0002022	.0000750	-.0000160
ζ_7	26373.562	.0021758	-.0006619	.0002450	-.0000524
ζ_8	10313.722	.0064699	-.0019759	.0007332	-.0001569
ζ_9	4295.2047	.0177005	-.0054633	.0020252	-.0004333
ζ_{10}	1883.2040	.0445108	-.0140337	.0052295	-.0011193
ζ_{11}	860.25938	.1013006	-.0334507	.0124929	-.0026755
ζ_{12}	405.70321	.1993058	-.0720251	.0272974	-.0058549
ζ_{13}	196.00495	.3088648	-.1336931	.0515611	-.0110884
ζ_{14}	96.392186	.3088528	-.1829556	.0741488	-.0160367
ζ_{15}	48.010429	.1418000	-.1017936	.0430262	-.0093797
ζ_{16}	24.124310	.0168419	.2227161	-.1075442	.0238160
ζ_{17}	12.193697	.0015377	.5564085	-.3802337	.0882915
ζ_{18}	6.1867732	-.0004640	.3524619	-.3507451	.0849577
ζ_{19}	3.1463420	.0003559	.0482718	.2018200	-.0585244
ζ_{20}	1.6022734	-.0003288	.0066118	.6061397	-.1838355
ζ_{21}	.81655825	.0002019	-.0015899	.4249718	-.2183978
ζ_{22}	.41629091	-.0001429	.0017834	.0716312	-.1032551
ζ_{23}	.21226448	.0000900	-.0010853	.0046617	.1426286
ζ_{24}	.10823916	-.0000505	.0006250	-.0015764	.4314802
ζ_{25}	.05519496	.0000220	-.0002755	.0008074	.4503415
ζ_{26}	.02814596	-.0000054	.0000684	-.0002119	.1704698

Table 26. Fe ^{5}D (26s, 17p, 13d; 26 ζ) (continued)

	Orbital	2p	3p		3d
	Energy	-27.41365	-2.74216		-0.64686
ζ_7	26373.562	.0000160	-.0000058		
ζ_8	10313.722	.0000508	-.0000183		
ζ_9	4295.2047	.0002476	-.0000898		
ζ_{10}	1883.2040	.0009489	-.0003436		
ζ_{11}	860.25938	.0034582	-.0012599		
ζ_{12}	405.70321	.0115360	-.0042213	ζ_{12}	.0001888
ζ_{13}	196.00495	.0347656	-.0129162	ζ_{13}	.0005109
ζ_{14}	96.392186	.0929124	-.0353579	ζ_{14}	.0025772
ζ_{15}	48.010429	.2017955	-.0797819	ζ_{15}	.0092594
ζ_{16}	24.124310	.3289316	-.1365302	ζ_{16}	.0288415
ζ_{17}	12.193697	.3372023	-.1440943	ζ_{17}	.0748648
ζ_{18}	6.1867732	.1556925	.0319364	ζ_{18}	.1601155
ζ_{19}	3.1463420	.0226867	.3142838	ζ_{19}	.2483141
ζ_{20}	1.6022734	.0021209	.4264516	ζ_{20}	.2879160
ζ_{21}	.81655825	.0001108	.2879913	ζ_{21}	.2610063
ζ_{22}	.41629091	.0002151	.0757545	ζ_{22}	.1805282
ζ_{23}	.21226448	-.0000296	.0097981	ζ_{23}	.0814357
ζ_{24}	.10823916			ζ_{24}	.0225938

Table 27. Co ^{4}F (26s, 17p, 13d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	17	13
Nuclear charge	27	Number of closed shells	4	2	0
No. of electrons	27	Open-shell occupation	0	0	7

Coupling coefficients

$K_0^{dd} = -0.08571429 \quad K_2^{dd} = -0.01449396 \quad K_4^{dd} = -0.00283215$

Total energy	Potential energy	Kinetic energy	Virial theorem
-1381.414509	-2762.829320	1381.414810	-1.99999978

	Orbital	1s	2s	3s	4s
	Energy	-283.06545	-34.86829	-4.52425	-0.26741
ζ_1	60672000.	.0000003	-.0000001	.0000000	.0000000
ζ_2	12604766.	.0000016	-.0000005	.0000002	.0000000
ζ_3	2989439.3	.0000092	-.0000028	.0000010	-.0000002
ζ_4	801967.00	.0000435	-.0000133	.0000049	-.0000010
ζ_5	240777.77	.0001791	-.0000546	.0000203	-.0000043
ζ_6	79956.482	.0006508	-.0001986	.0000741	-.0000156
ζ_7	29002.418	.0021246	-.0006496	.0002419	-.0000509
ζ_8	11345.405	.0063142	-.0019379	.0007235	-.0001523
ζ_9	4727.0836	.0172725	-.0053571	.0019979	-.0004206
ζ_{10}	2073.2941	.0434771	-.0137687	.0051620	-.0010872
ζ_{11}	947.14203	.0992263	-.0328911	.0123578	-.0026043
ζ_{12}	446.51595	.1963153	-.0711167	.0271158	-.0057231
ζ_{13}	215.54642	.3071317	-.1329593	.0515832	-.0109159
ζ_{14}	105.86859	.3118840	-.1842495	.0751184	-.0159866
ζ_{15}	52.642620	.1462267	-.1065277	.0453908	-.0097389
ζ_{16}	26.398883	.0177166	.2205881	-.1076146	.0234643
ζ_{17}	13.313028	.0015515	.5602650	-.3866251	.0883587
ζ_{18}	6.7379461	-.0004926	.3530977	-.3508115	.0835746
ζ_{19}	3.4176523	.0003773	.0474752	.2134923	-.0606659
ζ_{20}	1.7357011	-.0003431	.0066313	.6100541	-.1831664
ζ_{21}	.88209546	.0002134	-.0016428	.4164383	-.2128554
ζ_{22}	.44843609	-.0001503	.0018019	.0679435	-.0967225
ζ_{23}	.22800723	.0000948	-.0010969	.0046094	.1413508
ζ_{24}	.11593649	-.0000532	.0006318	-.0016013	.4253948
ζ_{25}	.05895199	.0000232	-.0002789	.0008189	.4465194
ζ_{26}	.02997631	-.0000058	.0000694	-.0002149	.1776447

Table 27. Co ^{4}F (26s, 17p, 13d; 26 ζ) (continued)

	Orbital	2p	3p		3d
	Energy	-30.12013	-3.00621		-0.67539
ζ_7	29002.418	.0000156	-.0000057		
ζ_8	11345.405	.0000496	-.0000181		
ζ_9	4727.0836	.0002414	-.0000884		
ζ_{10}	2073.2941	.0009256	-.0003384		
ζ_{11}	947.14203	.0033772	-.0012421		
ζ_{12}	446.51595	.0113060	-.0041770	ζ_{12}	.0001905
ζ_{13}	215.54642	.0342399	-.0128426	ζ_{13}	.0005206
ζ_{14}	105.86859	.0921362	-.0354085	ζ_{14}	.0026319
ζ_{15}	52.642620	.2017103	-.0805824	ζ_{15}	.0095466
ζ_{16}	26.398883	.3308891	-.1389614	ζ_{16}	.0299964
ζ_{17}	13.313028	.3384726	-.1454844	ζ_{17}	.0783520
ζ_{18}	6.7379461	.1541799	.0375329	ζ_{18}	.1661277
ζ_{19}	3.4176523	.0219367	.3226178	ζ_{19}	.2530516
ζ_{20}	1.7357011	.0021303	.4270436	ζ_{20}	.2875276
ζ_{21}	.88209546	.0001287	.2806259	ζ_{21}	.2561900
ζ_{22}	.44843609	.0002219	.0715256	ζ_{22}	.1759292
ζ_{23}	.22800723	-.0000265	.0090462	ζ_{23}	.0795998
ζ_{24}	.11593649			ζ_{24}	.0224874

Table 28. Ni ^{3}F (26s, 17p, 13d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	17	13
Nuclear charge	28	Number of closed shells	4	2	0
No. of electrons	28	Open-shell occupation	0	0	8

Coupling coefficients

$K_0^{dd} = -0.05000000$ $K_2^{dd} = -0.00663265$ $K_4^{dd} = 0.00229592$

Total energy	Potential energy	Kinetic energy	Virial theorem
-1506.870857	-3013.740490	1506.869640	-2.00000080

	Orbital	1s	2s	3s	4s
	Energy	-305.61908	-37.91787	-4.88784	-0.27624
ζ_1	67393769.	.0000003	-.0000001	.0000000	.0000000
ζ_2	13930933.	.0000016	-.0000005	.0000002	.0000000
ζ_3	3292307.1	.0000090	-.0000028	.0000010	-.0000002
ζ_4	881220.23	.0000424	-.0000130	.0000049	-.0000010
ζ_5	264240.98	.0001749	-.0000536	.0000201	-.0000042
ζ_6	87702.120	.0006355	-.0001948	.0000730	-.0000151
ζ_7	31809.669	.0020743	-.0006372	.0002385	-.0000494
ζ_8	12445.101	.0061647	-.0019006	.0007133	-.0001477
ζ_9	5185.8136	.0168712	-.0052560	.0019702	-.0004081
ζ_{10}	2274.3173	.0425299	-.0135231	.0050961	-.0010561
ζ_{11}	1038.5971	.0973616	-.0323860	.0122303	-.0025360
ζ_{12}	489.28600	.1936687	-.0703159	.0269474	-.0055961
ζ_{13}	235.94339	.3056265	-.1323466	.0516058	-.0107454
ζ_{14}	115.72624	.3145978	-.1854486	.0759898	-.0159115
ζ_{15}	57.447897	.1501774	-.1107055	.0474997	-.0100303
ζ_{16}	28.753468	.0184949	.2190784	-.1078893	.0231612
ζ_{17}	14.469995	.0015603	.5638617	-.3925239	.0882716
ζ_{18}	7.3071106	-.0005177	.3532270	-.3501826	.0820482
ζ_{19}	3.6976900	.0003963	.0466537	.2242911	-.0625058
ζ_{20}	1.8734163	-.0003554	.0066353	.6128662	-.1819333
ζ_{21}	.94976189	.0002234	-.0016831	.4087352	-.2074483
ζ_{22}	.48164829	-.0001566	.0018129	.0648886	-.0910994
ζ_{23}	.24428887	.0000988	-.0011035	.0045625	.1388838
ζ_{24}	.12390783	-.0000554	.0006356	-.0016167	.4192165
ζ_{25}	.06284924	.0000243	-.0002809	.0008258	.4428238
ζ_{26}	.03187884	-.0000060	.0000701	-.0002168	.1861534

Table 28. Ni ^{3}F (26s, 17p, 13d; 26 ζ) (continued)

	Orbital	2p	3p		3d
	Energy	-32.94177	-3.27768		-0.70693
ζ_7	31809.669	.0000152	-.0000056		
ζ_8	12445.101	.0000484	-.0000178		
ζ_9	5185.8136	.0002354	-.0000869		
ζ_{10}	2274.3173	.0009039	-.0003332		
ζ_{11}	1038.5971	.0033038	-.0012250		
ζ_{12}	489.28600	.0111030	-.0041363	ζ_{12}	.0001919
ζ_{13}	235.94339	.0337891	-.0127782	ζ_{13}	.0005295
ζ_{14}	115.72624	.0915087	-.0354693	ζ_{14}	.0026830
ζ_{15}	57.447897	.2017839	-.0813460	ζ_{15}	.0098181
ζ_{16}	28.753468	.3328079	-.1412152	ζ_{16}	.0310931
ζ_{17}	14.469995	.3394773	-.1465587	ζ_{17}	.0816293
ζ_{18}	7.3071106	.1525844	.0429852	ζ_{18}	.1716144
ζ_{19}	3.6976900	.0212402	.3300436	ζ_{19}	.2572171
ζ_{20}	1.8734163	.0021373	.4270623	ζ_{20}	.2871173
ζ_{21}	.94976189	.0001466	.2739729	ζ_{21}	.2519138
ζ_{22}	.48164829	.0002264	.0679585	ζ_{22}	.1716434
ζ_{23}	.24428887	-.0000236	.0084366	ζ_{23}	.0776691
ζ_{24}	.12390783			ζ_{24}	.0221981

Table 29. Cu ^{2}S (26s, 17p, 14d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	17	14
Nuclear charge	29	Number of closed shells	3	2	1
No. of electrons	29	Open-shell occupation	1	0	0

Coupling coefficients
$K_0^{ss} = -1.00000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-1638.963687	-3277.927300	1638.963610	-2.00000005

	Orbital	1s	2s	3s	4s
	Energy	-328.79296	-40.81894	-5.01196	-0.23848
ζ_1	32285234.	.0000008	-.0000002	.0000001	.0000000
ζ_2	6610569.9	.0000044	-.0000013	.0000005	-.0000001
ζ_3	1564955.3	.0000247	-.0000076	.0000028	-.0000005
ζ_4	423553.20	.0001143	-.0000352	.0000131	-.0000023
ζ_5	129366.36	.0004574	-.0001408	.0000527	-.0000091
ζ_6	43958.952	.0016025	-.0004939	.0001847	-.0000320
ζ_7	16371.703	.0050170	-.0015520	.0005814	-.0001008
ζ_8	6583.7187	.0142351	-.0044407	.0016623	-.0002882
ζ_9	2818.2848	.0368358	-.0117112	.0044032	-.0007640
ζ_{10}	1267.5889	.0861587	-.0284950	.0107374	-.0018632
ζ_{11}	592.24326	.1758761	-.0630178	.0240576	-.0041818
ζ_{12}	284.69694	.2896233	-.1214349	.0471011	-.0082010
ζ_{13}	139.71616	.3249114	-.1815318	.0736432	-.0128964
ζ_{14}	69.573562	.1823811	-.1387895	.0590806	-.0104001
ζ_{15}	34.992106	.0306601	.1435359	-.0682334	.0121468
ζ_{16}	17.715542	.0017888	.5301758	-.3436892	.0639353
ζ_{17}	9.0065037	-.0003104	.4245763	-.4031141	.0781937
ζ_{18}	4.5905463	.0003346	.0796000	.1015345	-.0248900
ζ_{19}	2.3432167	-.0003277	.0085275	.5621247	-.1330824
ζ_{20}	1.1970399	.0002068	-.0015167	.4812725	-.1573420
ζ_{21}	.61175889	-.0001543	.0021793	.1298564	-.1091852
ζ_{22}	.31270310	.0001035	-.0013765	.0082378	.0020124
ζ_{23}	.15985137	-.0000656	.0009146	.0001249	.2048445
ζ_{24}	.08171681	.0000367	-.0005193	.0004066	.4483637
ζ_{25}	.04177430	-.0000160	.0002269	-.0000618	.3906200
ζ_{26}	.02135539	.0000039	-.0000566	.0000595	.0885685

Table 29. Cu ^{2}S (26s, 17p, 14d; 26 ζ) (continued)

	Orbital	2p	3p		3d
	Energy	-35.61793	-3.32480		-0.49122
ζ_6	43958.952	.0000100	-.0000037		
ζ_7	16371.703	.0000367	-.0000135		
ζ_8	6583.7187	.0001823	-.0000673		
ζ_9	2818.2848	.0007294	-.0002685		
ζ_{10}	1267.5889	.0027225	-.0010092		
ζ_{11}	592.24326	.0092793	-.0034502	ζ_{11}	.0001474
ζ_{12}	284.69694	.0286267	-.0108018	ζ_{12}	.0004145
ζ_{13}	139.71616	.0787885	-.0303803	ζ_{13}	.0021030
ζ_{14}	69.573562	.1797257	-.0720491	ζ_{14}	.0078143
ζ_{15}	34.992106	.3119957	-.1311017	ζ_{15}	.0253730
ζ_{16}	17.715542	.3520780	-.1546022	ζ_{16}	.0679294
ζ_{17}	9.0065037	.1889073	-.0059112	ζ_{17}	.1479056
ζ_{18}	4.5905463	.0338694	.2794867	ζ_{18}	.2327667
ζ_{19}	2.3432167	.0032390	.4173447	ζ_{19}	.2699880
ζ_{20}	1.1970399	.0002786	.3171011	ζ_{20}	.2517864
ζ_{21}	.61175889	.0003380	.1092828	ζ_{21}	.1963950
ζ_{22}	.31270310	.0000146	.0185994	ζ_{22}	.1266079
ζ_{23}	.15985137			ζ_{23}	.0568967
ζ_{24}	.08171681			ζ_{24}	.0156562

Table 30. Zn ^{1}S (26s, 17p, 14d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	17	14
Nuclear charge	30	Number of closed shells	4	2	1
No. of electrons	30	Open-shell occupation	0	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-1777.848068	-3555.698240	1777.850170	-1.99999882

	Orbital	1s	2s	3s	4s
	Energy	-353.30436	-44.36156	-5.63772	-0.29249
ζ_1	68088788.	.0000003	-.0000001	.0000000	.0000000
ζ_2	13880630.	.0000019	-.0000006	.0000002	.0000000
ζ_3	3241320.5	.0000110	-.0000034	.0000013	-.0000003
ζ_4	859030.61	.0000524	-.0000162	.0000061	-.0000012
ζ_5	255624.88	.0002180	-.0000674	.0000254	-.0000051
ζ_6	84392.138	.0007960	-.0002460	.0000929	-.0000186
ζ_7	30517.316	.0026005	-.0008060	.0003044	-.0000610
ζ_8	11930.122	.0077037	-.0023976	.0009067	-.0001816
ζ_9	4977.4883	.0209100	-.0065928	.0024944	-.0004998
ζ_{10}	2189.6622	.0518962	-.0167571	.0063670	-.0012760
ζ_{11}	1004.5591	.1156727	-.0394299	.0150582	-.0030210
ζ_{12}	476.03982	.2199278	-.0830195	.0321752	-.0064639
ζ_{13}	231.14044	.3210102	-.1487936	.0590892	-.0119150
ζ_{14}	114.24067	.2882511	-.1860503	.0778030	-.0157749
ζ_{15}	57.178122	.1101448	-.0631003	.0280287	-.0057671
ζ_{16}	28.866111	.0093588	.3141511	-.1676488	.0351669
ζ_{17}	14.656461	.0011432	.5666623	-.4352015	.0956215
ζ_{18}	7.4687591	-.0004327	.2677684	-.2554344	.0574820
ζ_{19}	3.8143902	.0002658	.0278227	.3362652	-.0893219
ζ_{20}	1.9505199	-.0002409	.0039569	.6062498	-.1828869
ζ_{21}	.99808774	.0001470	-.0003816	.3344648	-.1872194
ζ_{22}	.51089338	-.0001022	.0006861	.0422627	-.0601701
ζ_{23}	.26154957	.0000642	-.0003717	.0038899	.1512547
ζ_{24}	.13390619	-.0000359	.0002114	-.0015553	.4133410
ζ_{25}	.06855733	.0000156	-.0000916	.0007584	.4196804
ζ_{26}	.03510011	-.0000038	.0000225	-.0001943	.1926402

Table 30. Zn ^{1}S (26s, 17p, 14d; 26 ζ) (continued)

	Orbital	2p	3p		3d
	Energy	-38.92468	-3.83928		-0.78245
ζ_7	30517.316	.0000212	-.0000079		
ζ_8	11930.122	.0000673	-.0000252		
ζ_9	4977.4883	.0003266	-.0001218		
ζ_{10}	2189.6622	.0012377	-.0004641		
ζ_{11}	1004.5591	.0044605	-.0016743	ζ_{11}	.0000588
ζ_{12}	476.03982	.0146376	-.0055526	ζ_{12}	.0001793
ζ_{13}	231.14044	.0433069	-.0166619	ζ_{13}	.0009435
ζ_{14}	114.24067	.1122170	-.0445619	ζ_{14}	.0037676
ζ_{15}	57.178122	.2322831	-.0959584	ζ_{15}	.0138090
ζ_{16}	28.866111	.3503056	-.1536897	ζ_{16}	.0410451
ζ_{17}	14.656461	.3062386	-.1234060	ζ_{17}	.1027178
ζ_{18}	7.4687591	.1104438	.1091949	ζ_{18}	.1962332
ζ_{19}	3.8143902	.0128446	.3689377	ζ_{19}	.2677064
ζ_{20}	1.9505199	.0013403	.4063945	ζ_{20}	.2782651
ζ_{21}	.99808774	.0003714	.2273596	ζ_{21}	.2310187
ζ_{22}	.51089338	.0000749	.0486017	ζ_{22}	.1503698
ζ_{23}	.26154957	.0000174	.0060518	ζ_{23}	.0654579
ζ_{24}	.13390619			ζ_{24}	.0179814

Table 31. Ga ^{2}P (26s, 20p, 14d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	20	14
Nuclear charge	31	Number of closed shells	4	2	1
No. of electrons	31	Open-shell occupation	0	1	0

Coupling coefficients

$K_0^{pp} = -1.66666667$ $K_2^{pp} = 0.13333333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-1923.260947	-3846.522830	1923.261890	-1.99999951

	Orbital	1s	2s	3s	4s
	Energy	-378.81829	-48.16830	-6.39455	-0.42453
ζ_1	73580197.	.0000003	-.0000001	.0000000	.0000000
ζ_2	14657018.	.0000020	-.0000006	.0000002	-.0000001
ζ_3	3366679.4	.0000115	-.0000036	.0000014	-.0000003
ζ_4	882769.12	.0000554	-.0000172	.0000065	-.0000015
ζ_5	261136.41	.0002313	-.0000717	.0000274	-.0000064
ζ_6	86013.253	.0008446	-.0002620	.0000999	-.0000233
ζ_7	31108.466	.0027532	-.0008567	.0003269	-.0000760
ζ_8	12179.866	.0081276	-.0025395	.0009697	-.0002257
ζ_9	5091.6945	.0219781	-.0069624	.0026619	-.0006194
ζ_{10}	2243.6525	.0543340	-.0176420	.0067694	-.0015763
ζ_{11}	1030.2315	.1205354	-.0414215	.0159958	-.0037267
ζ_{12}	488.10734	.2272807	-.0868568	.0340234	-.0079449
ζ_{13}	236.67348	.3258224	-.1542870	.0621188	-.0145508
ζ_{14}	116.68121	.2808820	-.1864815	.0790389	-.0186562
ζ_{15}	58.193673	.0986704	-.0439555	.0201016	-.0047872
ζ_{16}	29.250467	.0070354	.3560362	-.1982726	.0485186
ζ_{17}	14.776939	.0009998	.5643670	-.4559493	.1177275
ζ_{18}	7.4886157	-.0003943	.2292518	-.2020604	.0518950
ζ_{19}	3.8021330	.0002139	.0205534	.4080154	-.1257179
ζ_{20}	1.9324333	-.0001955	.0026628	.6138945	-.2367799
ζ_{21}	.98268876	.0001175	.0001498	.2725856	-.2217871
ζ_{22}	.49984826	-.0000805	.0001487	.0195662	.0061261
ζ_{23}	.25427675	.0000506	-.0000494	.0035431	.3351907
ζ_{24}	.12935744	-.0000282	.0000201	-.0016897	.5003783
ζ_{25}	.06580829	.0000123	-.0000090	.0008235	.2975108
ζ_{26}	.03347886	-.0000030	.0000017	-.0001949	.0445761

Table 31. Ga ^{2}P (26s, 20p, 14d; 26 ζ) (continued)

	Orbital	2p	3p	4p		3d
	Energy	-42.49390	-4.48227	-0.20850		-1.19327
ζ_7	31108.466	.0000232	-.0000088	.0000014		
ζ_8	12179.866	.0000730	-.0000278	.0000046		
ζ_9	5091.6945	.0003541	-.0001338	.0000218		
ζ_{10}	2243.6525	.0013360	-.0005090	.0000835		
ζ_{11}	1030.2315	.0048106	-.0018316	.0002990	ζ_{11}	.0000693
ζ_{12}	488.10734	.0157661	-.0060786	.0009974	ζ_{12}	.0002114
ζ_{13}	236.67348	.0466415	-.0182338	.0029869	ζ_{13}	.0011154
ζ_{14}	116.68121	.1202355	-.0486419	.0080172	ζ_{14}	.0044689
ζ_{15}	58.193673	.2457329	-.1034969	.0170843	ζ_{15}	.0163290
ζ_{16}	29.250467	.3591835	-.1611939	.0269065	ζ_{16}	.0483622
ζ_{17}	14.776939	.2917991	-.1107937	.0177892	ζ_{17}	.1195131
ζ_{18}	7.4886157	.0926796	.1482157	-.0296766	ζ_{18}	.2197733
ζ_{19}	3.8021330	.0096149	.3984720	-.0786412	ζ_{19}	.2870368
ζ_{20}	1.9324333	.0009084	.4004567	-.0844387	ζ_{20}	.2844174
ζ_{21}	.98268876	.0004472	.1871286	-.0480009	ζ_{21}	.2148730
ζ_{22}	.49984826	-.0000881	.0291248	.0638389	ζ_{22}	.1118801
ζ_{23}	.25427675	.0000962	.0027856	.2021016	ζ_{23}	.0327704
ζ_{24}	.12935744	-.0000571	.0000053	.3675221	ζ_{24}	.0045689
ζ_{25}	.06580829	.0000260	.0002813	.3261003		
ζ_{26}	.03347886	-.0000075	-.0000352	.2036763		

Table 32. Ge ^{3}P (26s, 20p, 14d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	20	14
Nuclear charge	32	Number of closed shells	4	2	1
No. of electrons	32	Open-shell occupation	0	2	0

Coupling coefficients

$K_0^{pp} = -0.66666667$ $K_2^{pp} = -0.06666667$

Total energy	Potential energy	Kinetic energy	Virial theorem
-2075.359681	-4150.720680	2075.361000	-1.99999936

	Orbital	1s	2s	3s	4s
	Energy	-405.24432	-52.15022	-7.19091	-0.55332
ζ_1	83575245.	.0000003	-.0000001	.0000000	.0000000
ζ_2	16849738.	.0000018	-.0000005	.0000002	-.0000001
ζ_3	3896374.3	.0000103	-.0000032	.0000012	-.0000003
ζ_4	1024074.1	.0000498	-.0000155	.0000060	-.0000015
ζ_5	302677.26	.0002087	-.0000649	.0000250	-.0000064
ζ_6	99408.028	.0007661	-.0002384	.0000919	-.0000236
ζ_7	35817.178	.0025116	-.0007839	.0003021	-.0000775
ζ_8	13972.261	.0074529	-.0023356	.0009014	-.0002312
ζ_9	5825.1379	.0202344	-.0064218	.0024797	-.0006358
ζ_{10}	2563.7409	.0502142	-.0163140	.0063262	-.0016236
ζ_{11}	1177.9335	.1120211	-.0383679	.0149532	-.0038389
ζ_{12}	559.50325	.2139658	-.0809517	.0320154	-.0082394
ζ_{13}	272.48200	.3164437	-.1461006	.0591818	-.0152729
ζ_{14}	135.14650	.2934347	-.1874005	.0799081	-.0207858
ζ_{15}	67.904354	.1195618	-.0765013	.0347264	-.0090981
ζ_{16}	34.423430	.0114021	.2918305	-.1583689	.0425375
ζ_{17}	17.553805	.0012058	.5670863	-.4377332	.1241752
ζ_{18}	8.9849994	-.0004710	.2892345	-.2843284	.0824742
ζ_{19}	4.6095032	.0003065	.0335396	.3133684	-.1064332
ζ_{20}	2.3678688	-.0002757	.0043500	.6315230	-.2576623
ζ_{21}	1.2172076	.0001721	-.0005668	.3449473	-.2764897
ζ_{22}	.62592189	-.0001191	.0007900	.0347907	-.0156812
ζ_{23}	.32191423	.0000754	-.0004767	.0046177	.3561538
ζ_{24}	.16557091	-.0000419	.0002588	-.0020169	.5118602
ζ_{25}	.08515983	.0000183	-.0001167	.0010874	.2953082
ζ_{26}	.04380129	-.0000045	.0000279	-.0002474	.0450969

Table 32. Ge ^{3}P (26s, 20p, 14d; 26 ζ) (continued)

	Orbital	2p	3p	4p		3d
	Energy	-46.23604	-5.16151	-0.28733		-1.63481
ζ_7	35817.178	.0000204	-.0000078	.0000015		
ζ_8	13972.261	.0000651	-.0000251	.0000050		
ζ_9	5825.1379	.0003157	-.0001213	.0000239		
ζ_{10}	2563.7409	.0011948	-.0004613	.0000912		
ζ_{11}	1177.9335	.0042970	-.0016621	.0003277	ζ_{11}	.0000634
ζ_{12}	559.50325	.0140783	-.0055002	.0010879	ζ_{12}	.0001916
ζ_{13}	272.48200	.0416483	-.0165097	.0032650	ζ_{13}	.0010089
ζ_{14}	135.14650	.1082731	-.0442807	.0088006	ζ_{14}	.0040120
ζ_{15}	67.904354	.2262815	-.0963778	.0192118	ζ_{15}	.0147510
ζ_{16}	34.423430	.3466471	-.1567720	.0315520	ζ_{16}	.0441315
ζ_{17}	17.553805	.3114548	-.1310263	.0259076	ζ_{17}	.1107895
ζ_{18}	8.9849994	.1182077	.1009176	-.0256816	ζ_{18}	.2109726
ζ_{19}	4.6095032	.0146530	.3712804	-.0891178	ζ_{19}	.2863066
ζ_{20}	2.3678688	.0014574	.4211356	-.1080071	ζ_{20}	.2919767
ζ_{21}	1.2172076	.0003152	.2222669	-.0692874	ζ_{21}	.2208907
ζ_{22}	.62592189	.0000538	.0396314	.0681012	ζ_{22}	.1095034
ζ_{23}	.32191423	.0000034	.0036128	.2448392	ζ_{23}	.0293242
ζ_{24}	.16557091	-.0000041	-.0000178	.3913112	ζ_{24}	.0041197
ζ_{25}	.08515983	.0000002	.0003600	.3109679		
ζ_{26}	.04380129	-.0000007	-.0000504	.1477560		

Table 33. As ^{4}S (26s, 19p, 14d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	20	14
Nuclear charge	33	Number of closed shells	4	2	1
No. of electrons	33	Open-shell occupation	0	3	0

Coupling coefficients

$K_0^{pp} = -0.33333333$ $K_2^{pp} = -0.13333333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-2234.238607	-4468.478630	2234.240030	-1.99999936

	Orbital	1s	2s	3s	4s
	Energy	-432.58609	-56.30973	-8.02955	-0.68586
ζ_1	92628131.	.0000003	-.0000001	.0000000	.0000000
ζ_2	18914773.	.0000016	-.0000005	.0000002	-.0000001
ζ_3	4410892.9	.0000095	-.0000030	.0000012	-.0000003
ζ_4	1164823.3	.0000457	-.0000143	.0000056	-.0000015
ζ_5	344914.01	.0001914	-.0000597	.0000233	-.0000064
ζ_6	113254.38	.0007040	-.0002198	.0000857	-.0000236
ζ_7	40746.374	.0023150	-.0007246	.0002822	-.0000777
ζ_8	15864.439	.0068933	-.0021664	.0008450	-.0002328
ζ_9	6602.4447	.0187780	-.0059707	.0023290	-.0006415
ζ_{10}	2902.7472	.0467847	-.0152128	.0059610	-.0016434
ζ_{11}	1333.6138	.1049935	-.0358729	.0141158	-.0038926
ζ_{12}	634.15428	.2029680	-.0762003	.0304269	-.0084118
ζ_{13}	309.55218	.3080454	-.1394189	.0568897	-.0157674
ζ_{14}	154.06121	.3023399	-.1870339	.0802694	-.0224283
ζ_{15}	77.751242	.1376451	-.0993304	.0451705	-.0127056
ζ_{16}	39.622344	.0163194	.2418652	-.1292891	.0371909
ζ_{17}	20.324148	.0013285	.5596847	-.4188192	.1273550
ζ_{18}	10.469399	-.0004644	.3361675	-.3389757	.1065644
ζ_{19}	5.4071293	.0003387	.0483613	.2371234	-.0869654
ζ_{20}	2.7968947	-.0003115	.0055469	.6356350	-.2728686
ζ_{21}	1.4479339	.0001965	-.0008632	.3991193	-.3228126
ζ_{22}	.74990037	-.0001373	.0011236	.0491889	-.0299677
ζ_{23}	.38845433	.0000875	-.0007147	.0055716	.3748049
ζ_{24}	.20123686	-.0000484	.0003877	-.0020971	.5215258
ζ_{25}	.10425203	.0000211	-.0001766	.0012546	.2912765
ζ_{26}	.05400866	-.0000051	.0000420	-.0002747	.0431881

Table 33. As ^{4}S (26s, 19p, 14d; 26 ζ) (continued)

	Orbital	2p	3p	4p		3d
	Energy	-50.15364	-5.88062	-0.36946		-2.11259
ζ_7	40746.374	.0000183	-.0000071	.0000016		
ζ_8	15864.439	.0000587	-.0000229	.0000051		
ζ_9	6602.4447	.0002850	-.0001113	.0000248		
ζ_{10}	2902.7472	.0010811	-.0004232	.0000943		
ζ_{11}	1333.6138	.0038927	-.0015291	.0003405	ζ_{11}	.0000586
ζ_{12}	634.15428	.0127729	-.0050581	.0011287	ζ_{12}	.0001765
ζ_{13}	309.55218	.0378888	-.0152310	.0034013	ζ_{13}	.0009292
ζ_{14}	154.06121	.0993161	-.0410935	.0092157	ζ_{14}	.0036873
ζ_{15}	77.751242	.2115685	-.0911992	.0205343	ζ_{15}	.0136469
ζ_{16}	39.622344	.3357200	-.1532446	.0348062	ζ_{16}	.0412868
ζ_{17}	20.324148	.3241308	-.1441455	.0324909	ζ_{17}	.1050263
ζ_{18}	10.469399	.1392858	.0666529	-.0206782	ζ_{18}	.2052544
ζ_{19}	5.4071293	.0200718	.3489372	-.0954752	ζ_{19}	.2865787
ζ_{20}	2.7968947	.0019222	.4344286	-.1268916	ζ_{20}	.2982712
ζ_{21}	1.4479339	.0002454	.2475178	-.0876056	ζ_{21}	.2242867
ζ_{22}	.74990037	.0001426	.0475912	.0735407	ζ_{22}	.1056974
ζ_{23}	.38845433	-.0000576	.0042742	.2773868	ζ_{23}	.0262092
ζ_{24}	.20123686	.0000314	-.0001843	.4042464	ζ_{24}	.0036659
ζ_{25}	.10425203	-.0000163	.0003266	.2937442		
ζ_{26}	.05400866	.0000040	-.0001025	.1158213		

Table 34. Se ^{3}P (26s, 20p, 14d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	20	14
Nuclear charge	34	Number of closed shells	4	2	1
No. of electrons	34	Open-shell occupation	0	4	0

Coupling coefficients

$K_0^{pp} = -0.16666667$ $K_2^{pp} = -0.01666667$

Total energy	Potential energy	Kinetic energy	Virial theorem
-2399.867562	-4799.735790	2399.868230	-1.99999972

	Orbital	1s	2s	3s	4s
	Energy	-460.86734	-60.66881	-8.93206	-0.83735
ζ_1	97160301.	.0000003	-.0000001	.0000000	.0000000
ζ_2	20098751.	.0000016	-.0000005	.0000002	-.0000001
ζ_3	4734337.5	.0000093	-.0000029	.0000011	-.0000003
ζ_4	1259495.3	.0000445	-.0000139	.0000055	-.0000016
ζ_5	374814.41	.0001853	-.0000580	.0000228	-.0000067
ζ_6	123437.10	.0006802	-.0002130	.0000839	-.0000245
ζ_7	44468.139	.0022361	-.0007020	.0002762	-.0000807
ζ_8	17314.523	.0066673	-.0021013	.0008281	-.0002422
ζ_9	7200.0900	.0182082	-.0058045	.0022876	-.0006687
ζ_{10}	3161.2408	.0455298	-.0148356	.0058728	-.0017190
ζ_{11}	1450.0447	.1026801	-.0351236	.0139624	-.0040862
ζ_{12}	688.37797	.1998558	-.0750003	.0302488	-.0088801
ζ_{13}	335.49414	.3063792	-.1382169	.0569618	-.0167545
ζ_{14}	166.73876	.3055151	-.1878681	.0814022	-.0241682
ζ_{15}	84.048576	.1424506	-.1047133	.0481558	-.0143558
ζ_{16}	42.788823	.0174757	.2349418	-.1269451	.0387353
ζ_{17}	21.930461	.0013524	.5604078	-.4227694	.1370531
ζ_{18}	11.289288	-.0004792	.3420229	-.3481421	.1163684
ζ_{19}	5.8273326	.0003522	.0499905	.2377068	-.0916332
ζ_{20}	3.0128121	-.0003241	.0055778	.6526637	-.3082413
ζ_{21}	1.5590505	.0002063	-.0009335	.3921060	-.3534473
ζ_{22}	.80713105	-.0001435	.0011163	.0415288	.0207027
ζ_{23}	.41794260	.0000918	-.0007379	.0062838	.4421758
ζ_{24}	.21643308	-.0000507	.0003927	-.0023539	.5176933
ζ_{25}	.11208338	.0000221	-.0001809	.0014215	.2341615
ζ_{26}	.05804450	-.0000054	.0000429	-.0003079	.0258199

Table 34. Se ^{3}P (26s, 20p, 14d; 26 ζ) (continued)

	Orbital	2p	3p	4p		3d
	Energy	-54.26884	-6.66148	-0.40283		-2.64958
ζ_7	44468.139	.0000175	-.0000069	.0000017		
ζ_8	17314.523	.0000563	-.0000223	.0000054		
ζ_9	7200.0900	.0002740	-.0001085	.0000262		
ζ_{10}	3161.2408	.0010433	-.0004143	.0001001		
ζ_{11}	1450.0447	.0037713	-.0015023	.0003633	ζ_{11}	.0000586
ζ_{12}	688.37797	.0124359	-.0049954	.0012091	ζ_{12}	.0001781
ζ_{13}	335.49414	.0370826	-.0151157	.0036660	ζ_{13}	.0009407
ζ_{14}	166.73876	.0978032	-.0410455	.0099882	ζ_{14}	.0037532
ζ_{15}	84.048576	.2098834	-.0917794	.0224536	ζ_{15}	.0139804
ζ_{16}	42.788823	.3355627	-.1555250	.0383568	ζ_{16}	.0425846
ζ_{17}	21.930461	.3261674	-.1472666	.0361199	ζ_{17}	.1088117
ζ_{18}	11.289288	.1411041	.0666884	-.0230698	ζ_{18}	.2123670
ζ_{19}	5.8273326	.0203843	.3558435	-.1065377	ζ_{19}	.2951306
ζ_{20}	3.0128121	.0018949	.4415683	-.1449209	ζ_{20}	.3025689
ζ_{21}	1.5590505	.0002074	.2384758	-.0883732	ζ_{21}	.2141255
ζ_{22}	.80713105	.0001298	.0405369	.1155048	ζ_{22}	.0887388
ζ_{23}	.41794260	-.0000645	.0040283	.3168832	ζ_{23}	.0183796
ζ_{24}	.21643308	.0000302	-.0001491	.3916612	ζ_{24}	.0023522
ζ_{25}	.11208338	-.0000186	.0005354	.2614756		
ζ_{26}	.05804450	.0000036	-.0000579	.0941916		

Table 35. Br ^{2}P (26s, 20p, 14d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	20	14
Nuclear charge	35	Number of closed shells	4	2	1
No. of electrons	35	Open-shell occupation	0	5	0

Coupling coefficients

$K_0^{pp} = -0.06666667$ $K_2^{pp} = 0.00533333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-2572.441282	-5144.883190	2572.441910	-1.99999976

	Orbital	1s	2s	3s	4s
	Energy	-490.06028	-65.19990	-9.87185	-0.99265
ζ_1	104204020.	.0000003	-.0000001	.0000000	.0000000
ζ_2	21720406.	.0000016	-.0000005	.0000002	-.0000001
ζ_3	5142183.4	.0000090	-.0000028	.0000011	-.0000003
ζ_4	1371890.8	.0000429	-.0000135	.0000054	-.0000016
ζ_5	408698.68	.0001788	-.0000561	.0000223	-.0000068
ζ_6	134563.04	.0006573	-.0002064	.0000821	-.0000252
ζ_7	48423.268	.0021654	-.0006817	.0002709	-.0000830
ζ_8	18826.268	.0064727	-.0020456	.0008142	-.0002497
ζ_9	7816.8253	.0177193	-.0056623	.0022538	-.0006906
ζ_{10}	3427.7662	.0444127	-.0145019	.0057977	-.0017793
ζ_{11}	1571.1261	.1004279	-.0343911	.0138065	-.0042351
ζ_{12}	745.76315	.1962934	-.0736317	.0299862	-.0092308
ζ_{13}	363.65566	.3033535	-.1362926	.0567006	-.0174804
ζ_{14}	180.94743	.3078641	-.1877360	.0820739	-.0255633
ζ_{15}	91.371087	.1486423	-.1115639	.0517877	-.0161699
ζ_{16}	46.621464	.0195429	.2194509	-.1192605	.0380939
ζ_{17}	23.958156	.0013792	.5559294	-.4192566	.1428292
ζ_{18}	12.369564	-.0004599	.3565880	-.3661476	.1286209
ζ_{19}	6.4052411	.0003487	.0561235	.2154121	-.0863106
ζ_{20}	3.3226205	-.0003272	.0058541	.6620521	-.3334013
ζ_{21}	1.7252551	.0002087	-.0009442	.4034227	-.3824572
ζ_{22}	.89628435	-.0001452	.0011220	.0423716	.0463399
ζ_{23}	.46573585	.0000935	-.0007697	.0070199	.4745938
ζ_{24}	.24203248	-.0000514	.0004021	-.0024376	.5123584
ζ_{25}	.12578252	.0000225	-.0001875	.0015386	.2102445
ζ_{26}	.06536868	-.0000054	.0000441	-.0003262	.0208940

Table 35. Br ^{2}P (26s, 20p, 14d; 26 ζ) (continued)

	Orbital	2p	3p	4p		3d
	Energy	-58.55417	-7.47817	-0.45706		-3.22013
ζ_7	48423.268	.0000168	-.0000067	.0000017		
ζ_8	18826.268	.0000543	-.0000218	.0000056		
ζ_9	7816.8253	.0002646	-.0001062	.0000275		
ζ_{10}	3427.7662	.0010103	-.0004067	.0001052		
ζ_{11}	1571.1261	.0036577	-.0014768	.0003827	ζ_{11}	.0000586
ζ_{12}	745.76315	.0120752	-.0049160	.0012735	ζ_{12}	.0001781
ζ_{13}	363.65566	.0360540	-.0148932	.0038697	ζ_{13}	.0009410
ζ_{14}	180.94743	.0953068	-.0405249	.0105586	ζ_{14}	.0037506
ζ_{15}	91.371087	.2056644	-.0911294	.0238938	ζ_{15}	.0139923
ζ_{16}	46.621464	.3320495	-.1559464	.0412009	ζ_{16}	.0427563
ζ_{17}	23.958156	.3290312	-.1517415	.0399872	ζ_{17}	.1095973
ζ_{18}	12.369564	.1474118	.0578732	-.0225577	ζ_{18}	.2146313
ζ_{19}	6.4052411	.0223432	.3529318	-.1140463	ζ_{19}	.2994511
ζ_{20}	3.3226205	.0019968	.4485894	-.1612225	ζ_{20}	.3056080
ζ_{21}	1.7252551	.0001853	.2399393	-.0919331	ζ_{21}	.2079578
ζ_{22}	.89628435	.0001333	.0394084	.1410153	ζ_{22}	.0793856
ζ_{23}	.46573585	-.0000782	.0042833	.3376409	ζ_{23}	.0148947
ζ_{24}	.24203248	.0000322	.0000199	.3842359	ζ_{24}	.0019108
ζ_{25}	.12578252	-.0000232	.0007137	.2421620		
ζ_{26}	.06536868	.0000037	-.0000166	.0820229		

Table 36. Kr ^{1}S (26s, 20p, 14d; 26 ζ)

		Symmetry species	S	P	D
		Number of basis functions	26	20	14
Nuclear charge	36	Number of closed shells	4	3	1
No. of electrons	36	Open-shell occupation	0	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-2752.054927	-5504.110420	2752.055490	-1.99999980

	Orbital	1s	2s	3s	4s
	Energy	-520.16541	-69.90303	-10.84943	-1.15291
ζ_1	111199310.	.0000003	-.0000001	.0000000	.0000000
ζ_2	23409280.	.0000015	-.0000005	.0000002	-.0000001
ζ_3	5579605.1	.0000087	-.0000027	.0000011	-.0000004
ζ_4	1494615.6	.0000413	-.0000130	.0000052	-.0000017
ζ_5	446067.60	.0001719	-.0000541	.0000217	-.0000069
ζ_6	146885.58	.0006326	-.0001992	.0000800	-.0000255
ζ_7	52804.705	.0020891	-.0006593	.0002645	-.0000842
ζ_8	20496.845	.0062619	-.0019840	.0007972	-.0002541
ζ_9	8495.7195	.0171905	-.0055054	.0022123	-.0007045
ζ_{10}	3719.9372	.0432078	-.0141348	.0057047	-.0018199
ζ_{11}	1703.4031	.0980011	-.0335857	.0136104	-.0043387
ζ_{12}	808.33246	.1924278	-.0721171	.0296418	-.0094860
ζ_{13}	394.36173	.2999441	-.1341031	.0562872	-.0180331
ζ_{14}	196.47296	.3101466	-.1873174	.0825748	-.0267467
ζ_{15}	99.405303	.1554643	-.1187039	.0555629	-.0180213
ζ_{16}	50.851111	.0220456	.2019018	-.1101653	.0365038
ζ_{17}	26.211822	.0014165	.5494710	-.4133646	.1466135
ζ_{18}	13.579842	-.0004277	.3729699	-.3853601	.1410275
ζ_{19}	7.0582189	.0003380	.0638678	.1871153	-.0770948
ζ_{20}	3.6757392	-.0003260	.0062231	.6682358	-.3533962
ζ_{21}	1.9163573	.0002081	-.0009181	.4195059	-.4096670
ζ_{22}	.99967963	-.0001450	.0011138	.0455550	.0613542
ζ_{23}	.52163173	.0000941	-.0007944	.0078001	.4937504
ζ_{24}	.27221705	-.0000515	.0004065	-.0024774	.5096201
ζ_{25}	.14206344	.0000225	-.0001923	.0016460	.1982643
ζ_{26}	.07414005	-.0000054	.0000449	-.0003419	.0187895

Table 36. Kr ^{1}S (26s, 20p, 14d; 26 ζ) (continued)

	Orbital	2p	3p	4p		3d
	Energy	-63.00974	-8.33146	-0.52417		-3.82520
ζ_7	52804.705	.0000160	-.0000065	.0000018		
ζ_8	20496.845	.0000521	-.0000212	.0000057		
ζ_9	8495.7195	.0002544	-.0001035	.0000282		
ζ_{10}	3719.9372	.0009740	-.0003973	.0001079		
ζ_{11}	1703.4031	.0035335	-.0014457	.0003937	ζ_{11}	.0000580
ζ_{12}	808.33246	.0116804	-.0048180	.0013106	ζ_{12}	.0001765
ζ_{13}	394.36173	.0349237	-.0146154	.0039907	ζ_{13}	.0009331
ζ_{14}	196.47296	.0925272	-.0398448	.0109043	ζ_{14}	.0037140
ζ_{15}	99.405303	.2008297	-.0901286	.0248433	ζ_{15}	.0138733
ζ_{16}	50.851111	.3277294	-.1558659	.0432777	ζ_{16}	.0425202
ζ_{17}	26.211822	.3320007	-.1564823	.0434665	ζ_{17}	.1093758
ζ_{18}	13.579842	.1548771	.0469525	-.0207245	ζ_{18}	.2153001
ζ_{19}	7.0582189	.0248606	.3474581	-.1189960	ζ_{19}	.3023345
ζ_{20}	3.6757392	.0021344	.4556046	-.1752036	ζ_{20}	.3081812
ζ_{21}	1.9163573	.0001700	.2445120	-.0961094	ζ_{21}	.2035097
ζ_{22}	.99967963	.0001420	.0396244	.1589926	ζ_{22}	.0731191
ζ_{23}	.52163173	-.0000820	.0040278	.3521629	ζ_{23}	.0128916
ζ_{24}	.27221705	.0000442	-.0004709	.3796948	ζ_{24}	.0016857
ζ_{25}	.14206344	-.0000215	.0004564	.2281862		
ζ_{26}	.07414005	.0000058	-.0001159	.0727195		

Table 37. Rb ^{2}S (28s, 20p, 14d; 28 ζ)

Nuclear charge	37
No. of electrons	37

Symmetry species	S	P	D
Number of basis functions	28	20	14
Number of closed shells	4	3	1
Open-shell occupation	1	0	0

Coupling coefficients
$K_0^{ss} = -1.00000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-2938.357357	-5876.715000	2938.357640	-1.99999990

	Orbital	1s	2s	3s	4s	5s
	Energy	-551.45728	-75.04931	-12.13317	-1.52353	-0.13784
ζ_1	29578241.	.0000017	-.0000005	.0000002	-.0000001	.0000000
ζ_2	5724040.9	.0000100	-.0000032	.0000013	-.0000004	.0000001
ζ_3	1313587.3	.0000576	-.0000182	.0000074	-.0000025	.0000005
ζ_4	352085.76	.0002657	-.0000839	.0000340	-.0000115	.0000024
ζ_5	108312.63	.0010387	-.0003281	.0001328	-.0000449	.0000094
ζ_6	37523.353	.0035040	-.0011103	.0004502	-.0001521	.0000320
ζ_7	14356.736	.0104493	-.0033313	.0013499	-.0004561	.0000960
ζ_8	5953.0845	.0279779	-.0090633	.0036864	-.0012462	.0002624
ζ_9	2629.2669	.0673860	-.0225294	.0091815	-.0031050	.0006538
ζ_{10}	1218.3397	.1431535	-.0511842	.0211021	-.0071488	.0015054
ζ_{11}	584.89442	.2530165	-.1027844	.0429576	-.0145869	.0030729
ζ_{12}	288.00490	.3279989	-.1698634	.0738551	-.0252350	.0053190
ζ_{13}	144.33946	.2425021	-.1771452	.0808690	-.0278615	.0058792
ζ_{14}	73.206235	.0674460	.0217978	-.0100989	.0034264	-.0007235
ζ_{15}	37.420146	.0035914	.4387721	-.2869389	.1050553	-.0223124
ζ_{16}	19.222845	.0004259	.5218665	-.4855544	.1882579	-.0402395
ζ_{17}	9.9049069	-.0001152	.1647679	-.0961938	.0356933	-.0076256
ζ_{18}	5.1128283	-.0000222	.0141880	.5646740	-.2759704	.0605560
ζ_{19}	2.6418628	-.0000170	.0002051	.6043284	-.5021324	.1185502
ζ_{20}	1.3658201	.0000003	.0010424	.1281647	-.1337097	.0291155
ζ_{21}	.70630824	.0000033	-.0008627	.0105570	.4648487	-.1290365
ζ_{22}	.36530005	-.0000010	.0005674	-.0027356	.6032377	-.1905756
ζ_{23}	.18894191	.0000016	-.0004363	.0032662	.2406451	-.2003628
ζ_{24}	.09772723	-.0000010	.0002922	-.0021466	.0113963	-.0906697
ζ_{25}	.05054819	.0000007	-.0001861	.0014157	.0038005	.2943749
ζ_{26}	.02614546	-.0000004	.0001041	-.0008086	-.0016357	.6335525
ζ_{27}	.01352344	.0000002	-.0000450	.0003505	.0010336	.2768894
ζ_{28}	.00699484	.0000000	.0000110	-.0000863	-.0002075	.0101090

Table 37. Rb ^{2}S (28s, 20p, 14d; 28 ζ) (continued)

	Orbital	2p	3p	4p		3d
	Energy	-67.90619	-9.48766	-0.81005		-4.73226
ζ_5	108312.63	.0000052	-.0000022	.0000006		
ζ_6	37523.353	.0000232	-.0000095	.0000028		
ζ_7	14356.736	.0001202	-.0000497	.0000149		
ζ_8	5953.0845	.0005051	-.0002073	.0000619		
ζ_9	2629.2669	.0019365	-.0008036	.0002403	ζ_9	.0000259
ζ_{10}	1218.3397	.0067179	-.0027841	.0008318	ζ_{10}	.0000898
ζ_{11}	584.89442	.0212009	-.0089350	.0026776	ζ_{11}	.0004753
ζ_{12}	288.00490	.0600653	-.0257366	.0077262	ζ_{12}	.0020141
ζ_{13}	144.33946	.1454914	-.0649482	.0196217	ζ_{13}	.0080183
ζ_{14}	73.206235	.2763697	-.1291092	.0392538	ζ_{14}	.0271877
ζ_{15}	37.420146	.3602752	-.1790672	.0550875	ζ_{15}	.0767935
ζ_{16}	19.222845	.2447387	-.0683354	.0173127	ζ_{16}	.1742585
ζ_{17}	9.9049069	.0624989	.2357382	-.0908133	ζ_{17}	.2827796
ζ_{18}	5.1128283	.0056768	.4665330	-.1872516	ζ_{18}	.3277421
ζ_{19}	2.6418628	.0002808	.3523790	-.1687314	ζ_{19}	.2522633
ζ_{20}	1.3658201	.0003292	.0851534	.0892625	ζ_{20}	.1056800
ζ_{21}	.70630824	-.0001914	.0076723	.3607681	ζ_{21}	.0209297
ζ_{22}	.36530005	.0001106	-.0003619	.4341238	ζ_{22}	.0021981
ζ_{23}	.18894191	-.0000539	.0005279	.2365109		
ζ_{24}	.09772723	.0000150	-.0001630	.0573443		

Table 38. Sr ^{1}S (27s, 20p, 14d; 27 ζ)

		Symmetry species	S	P	D
		Number of basis functions	27	20	14
Nuclear charge	38	Number of closed shells	5	3	1
No. of electrons	38	Open-shell occupation	0	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-3131.545580	-6263.091170	3131.545590	-2.00000000

	Orbital	1s	2s	3s	4s	5s
	Energy	-583.68784	-80.39077	-13.47501	-1.89680	-0.17845
ζ_1	26639868.	.0000020	-.0000006	.0000003	-.0000001	.0000000
ζ_2	5227514.5	.0000119	-.0000038	.0000015	-.0000005	.0000001
ζ_3	1208174.9	.0000681	-.0000216	.0000088	-.0000031	.0000008
ζ_4	324404.44	.0003147	-.0000996	.0000407	-.0000145	.0000037
ζ_5	99602.033	.0012364	-.0003917	.0001600	-.0000569	.0000147
ζ_6	34364.350	.0041956	-.0013332	.0005454	-.0001941	.0000501
ζ_7	13084.361	.0125662	-.0040244	.0016458	-.0005850	.0001509
ζ_8	5401.0536	.0336221	-.0109607	.0045004	-.0016029	.0004135
ζ_9	2377.2799	.0802104	-.0271617	.0111845	-.0039789	.0010263
ζ_{10}	1099.4128	.1661129	-.0607467	.0253403	-.0090532	.0023363
ζ_{11}	527.58991	.2787926	-.1185034	.0502780	-.0179629	.0046359
ζ_{12}	260.06408	.3266920	-.1822974	.0809168	-.0292487	.0075591
ζ_{13}	130.63734	.2018599	-.1564561	.0733103	-.0265065	.0068525
ζ_{14}	66.475107	.0410585	.1074445	-.0566864	.0205525	-.0053168
ζ_{15}	34.116255	.0019408	.5105848	-.3647176	.1438900	-.0376107
ζ_{16}	17.605099	-.0001344	.4542074	-.4587579	.1879816	-.0493716
ζ_{17}	9.1154853	.0002064	.1046890	.0559761	-.0245570	.0063202
ζ_{18}	4.7291884	-.0002569	.0089915	.6627234	-.3856442	.1067789
ζ_{19}	2.4562955	.0001627	-.0010091	.5002051	-.5143843	.1540531
ζ_{20}	1.2765369	-.0001235	.0014357	.0634854	.0431429	-.0228748
ζ_{21}	.66361209	.0000916	-.0011899	.0112207	.6224367	-.2168798
ζ_{22}	.34502722	-.0000624	.0007868	-.0051452	.5390887	-.3136997
ζ_{23}	.17939736	.0000424	-.0005591	.0043202	.0966093	-.1729602
ζ_{24}	.09327967	-.0000267	.0003538	-.0027385	.0064711	.2086021
ζ_{25}	.04850207	.0000148	-.0001979	.0015571	-.0024862	.5501534
ζ_{26}	.02531212	-.0000063	.0000847	-.0006733	.0011937	.4353613
ζ_{27}	.01296473	.0000015	-.0000200	.0001596	-.0002989	.0645291

Table 38. Sr ^{1}S (27s, 20p, 14d; 27 ζ) (continued)

	Orbital	2p	3p	4p		3d
	Energy	-72.99602	-10.69996	-1.09815		-5.69438
ζ_5	99602.033	.0000066	-.0000028	.0000009		
ζ_6	34364.350	.0000301	-.0000125	.0000040		
ζ_7	13084.361	.0001563	-.0000652	.0000210		
ζ_8	5401.0536	.0006633	-.0002764	.0000885	ζ_8	.0000061
ζ_9	2377.2799	.0025374	-.0010634	.0003426	ζ_9	.0000266
ζ_{10}	1099.4128	.0087666	-.0036903	.0011843	ζ_{10}	.0001449
ζ_{11}	527.58991	.0272007	-.0116215	.0037522	ζ_{11}	.0006782
ζ_{12}	260.06408	.0751258	-.0328617	.0106107	ζ_{12}	.0028858
ζ_{13}	130.63734	.1730381	-.0788939	.0257145	ζ_{13}	.0111558
ζ_{14}	66.475107	.3059256	-.1471435	.0482104	ζ_{14}	.0360300
ζ_{15}	34.116255	.3520684	-.1755786	.0582389	ζ_{15}	.0974203
ζ_{16}	17.605099	.1973819	-.0098839	-.0041233	ζ_{16}	.2044519
ζ_{17}	9.1154853	.0392217	.3093432	-.1274192	ζ_{17}	.3050583
ζ_{18}	4.7291884	.0032399	.4782973	-.2208164	ζ_{18}	.3222082
ζ_{19}	2.4562955	.0000844	.2821078	-.1337630	ζ_{19}	.2125740
ζ_{20}	1.2765369	.0002503	.0482046	.1942248	ζ_{20}	.0697106
ζ_{21}	.66361209	-.0001648	.0047040	.4451367	ζ_{21}	.0115977
ζ_{22}	.34502722	.0000937	-.0008719	.3992235		
ζ_{23}	.17939736	-.0000444	.0005452	.1286856		
ζ_{24}	.09327967	.0000127	-.0001987	.0211925		

Table 39. Y ^{2}D (27s, 20p, 17d; 27 ζ)

		Symmetry species	S	P	D
		Number of basis functions	27	20	17
Nuclear charge	39	Number of closed shells	5	3	1
No. of electrons	39	Open-shell occupation	0	0	1

Coupling coefficients

$K_0^{dd} = -1.80000000$ $K_2^{dd} = 0.05714286$ $K_4^{dd} = 0.05714286$

Total energy	Potential energy	Kinetic energy	Virial theorem
-3331.684053	-6663.368130	3331.684080	-1.99999999

	Orbital	1s	2s	3s	4s	5s
	Energy	-616.74927	-85.81088	-14.75886	-2.16882	-0.19612
ζ_1	29642329.	.0000019	-.0000006	.0000002	-.0000001	.0000000
ζ_2	5766661.3	.0000113	-.0000036	.0000015	-.0000005	.0000001
ζ_3	1326534.1	.0000648	-.0000206	.0000085	-.0000031	.0000008
ζ_4	355629.43	.0002996	-.0000950	.0000392	-.0000144	.0000038
ζ_5	109262.64	.0011742	-.0003728	.0001535	-.0000565	.0000150
ζ_6	37772.140	.0039719	-.0012649	.0005218	-.0001921	.0000510
ζ_7	14416.863	.0118657	-.0038068	.0015696	-.0005772	.0001532
ζ_8	5964.0349	.0317384	-.0103580	.0042880	-.0015805	.0004197
ζ_9	2628.7927	.0759818	-.0257090	.0106701	-.0039264	.0010421
ζ_{10}	1216.1770	.1588859	-.0578732	.0243270	-.0089951	.0023897
ζ_{11}	583.16871	.2716668	-.1142613	.0488047	-.0180330	.0047886
ζ_{12}	286.91840	.3291254	-.1802303	.0804515	-.0301008	.0080109
ζ_{13}	143.71410	.2143695	-.1646929	.0775534	-.0289914	.0077068
ζ_{14}	72.860547	.0472406	.0863585	-.0454169	.0168443	-.0044627
ζ_{15}	37.232352	.0021360	.5019396	-.3571250	.1460151	-.0393602
ζ_{16}	19.121368	-.0000174	.4712431	-.4757664	.2019837	-.0546003
ζ_{17}	9.8500317	.0001325	.1128299	.0388053	-.0159738	.0039051
ζ_{18}	5.0830613	-.0002064	.0093002	.6790481	-.4183215	.1206047
ζ_{19}	2.6256642	.0001262	-.0010432	.5024481	-.5457913	.1691785
ζ_{20}	1.3569865	-.0000965	.0014187	.0568157	.1007570	-.0428494
ζ_{21}	.70148755	.0000728	-.0012024	.0118812	.6843476	-.2600643
ζ_{22}	.36267068	-.0000493	.0007961	-.0057916	.4895601	-.3304109
ζ_{23}	.18750979	.0000336	-.0005632	.0046640	.0626194	-.1077226
ζ_{24}	.09694869	-.0000211	.0003573	-.0029670	.0076111	.2837024
ζ_{25}	.05012584	.0000118	-.0002003	.0016863	-.0035044	.5704750
ζ_{26}	.02591683	-.0000051	.0000868	-.0007372	.0016565	.3576719
ζ_{27}	.01339991	.0000012	-.0000212	.0001807	-.0004194	.0387588

Table 39. Y ^{2}D (27s, 20p, 17d; 27 ζ) (continued)

	Orbital	2p	3p	4p		3d	4d
	Energy	-78.16441	-11.85413	-1.30114		-6.59942	-0.24985
ζ_5	109262.64	.0000062	-.0000026	.0000009			
ζ_6	37772.140	.0000280	-.0000118	.0000039			
ζ_7	14416.863	.0001449	-.0000611	.0000206			
ζ_8	5964.0349	.0006128	-.0002581	.0000864			
ζ_9	2628.7927	.0023448	-.0009934	.0003352	ζ_9	.0000355	-.0000076
ζ_{10}	1216.1770	.0081307	-.0034579	.0011605	ζ_{10}	.0001210	-.0000266
ζ_{11}	583.16871	.0254275	-.0109741	.0037101	ζ_{11}	.0006506	-.0001394
ζ_{12}	286.91840	.0710980	-.0313866	.0106006	ζ_{12}	.0027138	-.0005918
ζ_{13}	143.71410	.1668172	-.0767476	.0261948	ζ_{13}	.0107224	-.0023213
ζ_{14}	72.860547	.3017225	-.1464140	.0501994	ζ_{14}	.0352388	-.0077126
ζ_{15}	37.232352	.3571041	-.1806433	.0628623	ζ_{15}	.0970175	-.0213212
ζ_{16}	19.121368	.2063355	-.0191809	-.0011576	ζ_{16}	.2069150	-.0459112
ζ_{17}	9.8500317	.0417950	.3104429	-.1349138	ζ_{17}	.3116447	-.0667659
ζ_{18}	5.0830613	.0033553	.4888117	-.2406821	ζ_{18}	.3275857	-.0660846
ζ_{19}	2.6256642	.0000223	.2791003	-.1326115	ζ_{19}	.2058343	-.0087497
ζ_{20}	1.3569865	.0002665	.0431052	.2368314	ζ_{20}	.0617112	.1147591
ζ_{21}	.70148755	-.0001867	.0043813	.4791233	ζ_{21}	.0079676	.2413229
ζ_{22}	.36267068	.0001045	-.0010247	.3668823	ζ_{22}	.0002331	.3082091
ζ_{23}	.18750979	-.0000504	.0006012	.0957048	ζ_{23}	.0002197	.3039688
ζ_{24}	.09694869	.0000140	-.0002026	.0147509	ζ_{24}	-.0000659	.1872081
ζ_{25}	.05012584				ζ_{25}	.0000345	.0964297

Table 40. Zr ^{5}F (27s, 20p, 17d; 27 ζ)

		Symmetry species	S	P	D
		Number of basis functions	27	20	17
Nuclear charge	40	Number of closed shells	4	3	1
No. of electrons	40	Open-shell occupation	1	0	3

Coupling coefficients

$K_0^{ss} = -1.00000000$
$K_0^{dd} = -0.46666667 \quad K_2^{dd} = -0.07891156 \quad K_4^{dd} = -0.01541950$
$K_2^{sd} = -0.20000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-3539.009463	-7078.019120	3539.009650	-1.99999995

	Orbital	1s	2s	3s	4s	5s
	Energy	-650.59464	-91.26131	-15.93825	-2.30705	-0.20564
ζ_1	29410970.	.0000020	-.0000006	.0000003	-.0000001	.0000000
ζ_2	5715492.9	.0000121	-.0000039	.0000016	-.0000006	.0000002
ζ_3	1314110.7	.0000699	-.0000222	.0000092	-.0000035	.0000009
ζ_4	352263.05	.0003230	-.0001027	.0000426	-.0000160	.0000041
ζ_5	108238.80	.0012656	-.0004028	.0001672	-.0000628	.0000161
ζ_6	37422.134	.0042792	-.0013660	.0005677	-.0002135	.0000549
ζ_7	14282.590	.0127749	-.0041116	.0017089	-.0006415	.0001650
ζ_8	5906.6028	.0341139	-.0111760	.0046621	-.0017549	.0004516
ζ_9	2601.7622	.0813561	-.0277130	.0116016	-.0043579	.0011206
ζ_{10}	1202.4429	.1685772	-.0620685	.0263133	-.0099404	.0025595
ζ_{11}	575.79457	.2825947	-.1213948	.0524332	-.0197818	.0050893
ζ_{12}	282.81588	.3280709	-.1858430	.0839819	-.0321510	.0082964
ζ_{13}	141.38571	.1966353	-.1540224	.0739319	-.0281933	.0072559
ζ_{14}	71.527241	.0368415	.1314320	-.0724200	.0277922	-.0071443
ζ_{15}	36.467534	.0017047	.5350169	-.3996196	.1687757	-.0441947
ζ_{16}	18.683764	-.0002672	.4319525	-.4554986	.1982512	-.0519484
ζ_{17}	9.6008578	.0002693	.0850153	.1398237	-.0627942	.0160711
ζ_{18}	4.9420097	-.0002988	.0072600	.7296428	-.5051861	.1437344
ζ_{19}	2.5463037	.0001978	-.0014972	.4186900	-.5042634	.1521429
ζ_{20}	1.3125979	-.0001444	.0014771	.0297286	.2784348	-.1008771
ζ_{21}	.67679511	.0001062	-.0012390	.0106895	.7053994	-.2818820
ζ_{22}	.34900265	-.0000726	.0008262	-.0053114	.3829021	-.2833199
ζ_{23}	.17997757	.0000490	-.0005755	.0040805	.0363929	-.0549002
ζ_{24}	.09281415	-.0000309	.0003639	-.0025678	.0063177	.3298278
ζ_{25}	.04786429	.0000172	-.0002058	.0014314	-.0055531	.5837365
ζ_{26}	.02468365	-.0000074	.0000879	-.0006375	.0004634	.2903099
ζ_{27}	.01272938	.0000018	-.0000217	.0001540	-.0004743	.0207951

Table 40. Zr ^{5}F (27s, 20p, 17d; 27 ζ) (continued)

	Orbital	2p	3p	4p		3d	4d
	Energy	-83.36332	-12.90405	-1.38741		-7.40153	-0.25045
ζ_5	108238.80	.0000069	-.0000029	.0000010			
ζ_6	37422.134	.0000313	-.0000133	.0000046			
ζ_7	14282.590	.0001615	-.0000687	.0000238			
ζ_8	5906.6028	.0006842	-.0002917	.0001002			
ζ_9	2601.7622	.0026154	-.0011176	.0003865	ζ_9	.0000421	-.0000093
ζ_{10}	1202.4429	.0090693	-.0039060	.0013447	ζ_{10}	.0001428	-.0000321
ζ_{11}	575.79457	.0282643	-.0123281	.0042735	ζ_{11}	.0007740	-.0001711
ζ_{12}	282.81588	.0785073	-.0351814	.0121960	ζ_{12}	.0032136	-.0007194
ζ_{13}	141.38571	.1809369	-.0844581	.0295864	ζ_{13}	.0126523	-.0028222
ζ_{14}	71.527241	.3172354	-.1570919	.0553677	ζ_{14}	.0409655	-.0092244
ζ_{15}	36.467534	.3516113	-.1772236	.0631028	ζ_{15}	.1110332	-.0251773
ζ_{16}	18.683764	.1817917	.0176089	-.0167693	ζ_{16}	.2275603	-.0518874
ζ_{17}	9.6008578	.0312616	.3585047	-.1615005	ζ_{17}	.3273808	-.0717092
ζ_{18}	4.9420097	.0023912	.4884131	-.2582119	ζ_{18}	.3200093	-.0636148
ζ_{19}	2.5463037	-.0000605	.2280260	-.0781547	ζ_{19}	.1737292	.0153215
ζ_{20}	1.3125979	.0002103	.0261587	.3230398	ζ_{20}	.0416538	.1533697
ζ_{21}	.67679511	-.0001621	.0030722	.4830735	ζ_{21}	.0042607	.2649348
ζ_{22}	.34900265	.0000853	-.0007536	.3018792	ζ_{22}	.0001280	.3011629
ζ_{23}	.17997757	-.0000430	.0004719	.0679372	ζ_{23}	.0001745	.2789396
ζ_{24}	.09281415	.0000111	-.0001276	.0094938	ζ_{24}	-.0000387	.1730632
ζ_{25}	.04786429				ζ_{25}	.0000291	.0821049

Table 41. Nb ^{6}D (27s, 20p, 17d; 27 ζ)

		Symmetry species	S	P	D
		Number of basis functions	27	20	17
Nuclear charge	41	Number of closed shells	4	3	1
No. of electrons	41	Open-shell occupation	1	0	4

Coupling coefficients

$K_0^{ss} = -1.00000000$
$K_0^{dd} = -0.30000000 \quad K_2^{dd} = -0.05000000 \quad K_4^{dd} = -0.05000000$
$K_2^{sd} = -0.20000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-3753.597595	-7507.195300	3753.597710	-1.99999997

	Orbital	1s	2s	3s	4s	5s
	Energy	-685.44392	-96.97476	-17.24699	-2.53741	-0.21556
ζ_1	31685643.	.0000020	-.0000006	.0000003	-.0000001	.0000000
ζ_2	6210014.0	.0000116	-.0000037	.0000015	-.0000006	.0000002
ζ_3	1434125.3	.0000666	-.0000212	.0000089	-.0000034	.0000009
ζ_4	384892.20	.0003077	-.0000980	.0000410	-.0000158	.0000041
ζ_5	118137.71	.0012093	-.0003857	.0001613	-.0000619	.0000159
ζ_6	40748.257	.0041057	-.0013133	.0005498	-.0002114	.0000545
ζ_7	15509.361	.0123090	-.0039682	.0016613	-.0006376	.0001642
ζ_8	6398.5333	.0329919	-.0108232	.0045479	-.0017501	.0004511
ζ_9	2814.0926	.0789366	-.0268936	.0113389	-.0043544	.0011218
ζ_{10}	1300.0520	.1642328	-.0603803	.0257778	-.0099554	.0025679
ζ_{11}	623.05518	.2774561	-.1184864	.0515057	-.0198660	.0051204
ζ_{12}	306.64757	.3281309	-.1836460	.0834686	-.0326668	.0084447
ζ_{13}	153.76946	.2049079	-.1597421	.0770018	-.0300361	.0077469
ζ_{14}	78.097454	.0419160	.1086040	-.0596565	.0232440	-.0059779
ζ_{15}	40.000172	.0018899	.5176573	-.3830341	.1652877	-.0433783
ζ_{16}	20.597925	-.0001482	.4525024	-.4737188	.2111791	-.0555222
ζ_{17}	10.641987	.0002017	.1003348	.0870951	-.0372838	.0093051
ζ_{18}	5.5089630	-.0002552	.0080112	.7216628	-.5040395	.1436446
ζ_{19}	2.8549143	.0001655	-.0012077	.4559159	-.5456091	.1657429
ζ_{20}	1.4803640	-.0001226	.0013334	.0382473	.2548564	-.0940225
ζ_{21}	.76783605	.0000915	-.0011599	.0117643	.7081270	-.2865509
ζ_{22}	.39831330	-.0000625	.0007711	-.0058152	.4017032	-.2816097
ζ_{23}	.20663501	.0000424	-.0005421	.0045441	.0451659	-.0590111
ζ_{24}	.10719905	-.0000267	.0003427	-.0028636	.0062052	.2929405
ζ_{25}	.05561350	.0000148	-.0001950	.0016023	-.0056501	.5597068
ζ_{26}	.02885161	-.0000064	.0000818	-.0007108	-.0000562	.3340265
ζ_{27}	.01496786	.0000015	-.0000204	.0001706	-.0005389	.0365995

Table 41. Nb ^{6}D (27s, 20p, 17d; 27 ζ) (continued)

	Orbital	2p	3p	4p		3d	4d
	Energy	-88.82305	-14.08136	-1.55693		-8.32922	-0.30061
ζ_5	118137.71	.0000065	-.0000028	.0000010			
ζ_6	40748.257	.0000296	-.0000127	.0000045			
ζ_7	15509.361	.0001536	-.0000660	.0000235			
ζ_8	6398.5333	.0006532	-.0002810	.0000992			
ζ_9	2814.0926	.0025042	-.0010806	.0003844	ζ_9	.0000407	-.0000099
ζ_{10}	1300.0520	.0086879	-.0037753	.0013364	ζ_{10}	.0001384	-.0000343
ζ_{11}	623.05518	.0270895	-.0119261	.0042525	ζ_{11}	.0007479	-.0001823
ζ_{12}	306.64757	.0752777	-.0340138	.0121242	ζ_{12}	.0030971	-.0007642
ζ_{13}	153.76946	.1744046	-.0820901	.0295842	ζ_{13}	.0121716	-.0029933
ζ_{14}	78.097454	.3094776	-.1543413	.0559436	ζ_{14}	.0394926	-.0098061
ζ_{15}	40.000172	.3532785	-.1810829	.0664867	ζ_{15}	.1074537	-.0268802
ζ_{16}	20.597925	.1933554	-.0004279	-.0099191	ζ_{16}	.2227049	-.0560985
ζ_{17}	10.641987	.0364446	.3405978	-.1588090	ζ_{17}	.3254129	-.0788276
ζ_{18}	5.5089630	.0027224	.4946872	-.2692307	ζ_{18}	.3232385	-.0708992
ζ_{19}	2.8549143	-.0000274	.2449881	-.0950557	ζ_{19}	.1775579	.0164758
ζ_{20}	1.4803640	.0001992	.0303491	.3198313	ζ_{20}	.0426572	.1689458
ζ_{21}	.76783605	-.0001652	.0035313	.4844444	ζ_{21}	.0044140	.2839347
ζ_{22}	.39831330	.0000833	-.0008125	.3067893	ζ_{22}	.0001091	.3084783
ζ_{23}	.20663501	-.0000436	.0005457	.0725524	ζ_{23}	.0001979	.2636361
ζ_{24}	.10719905	.0000109	-.0001409	.0103196	ζ_{24}	-.0000502	.1517717
ζ_{25}	.05561350				ζ_{25}	.0000304	.0643725

Table 42. Mo ^{7}S (27s, 20p, 17d; 27 ζ)

		Symmetry species	S	P	D
		Number of basis functions	27	20	17
Nuclear charge	42	Number of closed shells	4	3	1
No. of electrons	42	Open-shell occupation	1	0	5

Coupling coefficients

$K_0^{ss} = -1.00000000$
$K_0^{dd} = -0.20000000 \quad K_2^{dd} = -0.05714286 \quad K_4^{dd} = -0.05714286$
$K_2^{sd} = -0.20000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-3975.549367	-7951.098900	3975.549530	-1.99999996

	Orbital	1s	2s	3s	4s	5s
	Energy	-721.20211	-102.85054	-18.58448	-2.76286	-0.22271
ζ_1	34840341.	.0000018	-.0000006	.0000002	-.0000001	.0000000
ζ_2	6830969.4	.0000109	-.0000035	.0000015	-.0000006	.0000001
ζ_3	1577505.4	.0000628	-.0000200	.0000084	-.0000033	.0000008
ζ_4	423261.18	.0002904	-.0000927	.0000390	-.0000153	.0000039
ζ_5	129869.03	.0011418	-.0003648	.0001536	-.0000600	.0000154
ζ_6	44781.924	.0038791	-.0012432	.0005241	-.0002052	.0000525
ζ_7	17043.131	.0116366	-.0037567	.0015835	-.0006189	.0001583
ζ_8	7032.7149	.0312281	-.0102535	.0043380	-.0017003	.0004352
ζ_9	3094.6786	.0749275	-.0255008	.0108212	-.0042321	.0010825
ζ_{10}	1430.9523	.1569545	-.0574730	.0246920	-.0097122	.0024872
ζ_{11}	686.62981	.2690889	-.1136361	.0496508	-.0195006	.0049904
ζ_{12}	338.45022	.3284732	-.1800367	.0821586	-.0327390	.0084024
ζ_{13}	170.01631	.2181565	-.1678853	.0810490	-.0322058	.0082503
ζ_{14}	86.518004	.0501656	.0774292	-.0420223	.0164003	-.0041733
ζ_{15}	44.406241	.0022727	.4942639	-.3598766	.1578382	-.0411280
ζ_{16}	22.917327	.0000345	.4787324	-.4937507	.2242865	-.0586221
ζ_{17}	11.867335	.0000921	.1208165	.0246926	-.0059571	.0009619
ζ_{18}	6.1575957	-.0001796	.0092699	.7088570	-.4952067	.1398226
ζ_{19}	3.1985876	.0001087	-.0008669	.4981330	-.5890973	.1782070
ζ_{20}	1.6625137	-.0000830	.0011619	.0483454	.2260047	-.0843101
ζ_{21}	.86437253	.0000640	-.0010582	.0130538	.7106123	-.2870915
ζ_{22}	.44946422	-.0000433	.0006990	-.0064177	.4208640	-.2781205
ζ_{23}	.23372924	.0000296	-.0004966	.0050845	.0537847	-.0645689
ζ_{24}	.12154561	-.0000186	.0003140	-.0032101	.0061956	.2587170
ζ_{25}	.06320739	.0000104	-.0001803	.0018072	-.0055316	.5341088
ζ_{26}	.03286979	-.0000045	.0000740	-.0007969	-.0004691	.3713141
ζ_{27}	.01709331	.0000011	-.0000189	.0001915	-.0006310	.0562579

Table 42. Mo ^{7}S (27s, 20p, 17d; 27 ζ) (continued)

	Orbital	2p	3p	4p		3d	4d
	Energy	-94.44403	-15.28651	-1.72359		-9.28417	-0.35789
ζ_5	129869.03	.0000060	-.0000026	.0000010			
ζ_6	44781.924	.0000274	-.0000119	.0000043			
ζ_7	17043.131	.0001424	-.0000618	.0000225			
ζ_8	7032.7149	.0006050	-.0002624	.0000947			
ζ_9	3094.6786	.0023206	-.0010107	.0003682	ζ_9	.0000377	-.0000098
ζ_{10}	1430.9523	.0080522	-.0035269	.0012770	ζ_{10}	.0001281	-.0000341
ζ_{11}	686.62981	.0251780	-.0111779	.0040805	ζ_{11}	.0006918	-.0001812
ζ_{12}	338.45022	.0703323	-.0319894	.0116637	ζ_{12}	.0028674	-.0007612
ζ_{13}	170.01631	.1650966	-.0782224	.0288572	ζ_{13}	.0113188	-.0029930
ζ_{14}	86.518004	.2994591	-.1500453	.0556297	ζ_{14}	.0371179	-.0099148
ζ_{15}	44.406241	.3564728	-.1857212	.0699816	ζ_{15}	.1022372	-.0275113
ζ_{16}	22.917327	.2091451	-.0228145	-.0007438	ζ_{16}	.2163411	-.0587447
ζ_{17}	11.867335	.0435378	.3188599	-.1530475	ζ_{17}	.3234978	-.0846229
ζ_{18}	6.1575957	.0032446	.5018884	-.2790844	ζ_{18}	.3285640	-.0779488
ζ_{19}	3.1985876	.0000020	.2651881	-.1149686	ζ_{19}	.1836582	.0156385
ζ_{20}	1.6625137	.0001948	.0351899	.3143624	ζ_{20}	.0442388	.1809383
ζ_{21}	.86437253	-.0001740	.0041393	.4868307	ζ_{21}	.0045956	.2989160
ζ_{22}	.44946422	.0000841	-.0009254	.3131779	ζ_{22}	.0000124	.3139131
ζ_{23}	.23372924	-.0000457	.0006505	.0770909	ζ_{23}	.0001886	.2513439
ζ_{24}	.12154561	.0000112	-.0001634	.0108960	ζ_{24}	-.0000932	.1354375
ζ_{25}	.06320739				ζ_{25}	.0000249	.0506689

Table 43. Tc ^{6}S (27s, 20p, 17d; 27 ζ)

Nuclear charge	43
No. of electrons	43

Symmetry species	S	P	D
Number of basis functions	27	20	17
Number of closed shells	5	3	1
Open-shell occupation	0	0	5

Coupling coefficients

$K_0^{dd} = -0.20000000$ $K_2^{dd} = -0.05714286$ $K_4^{dd} = -0.05714286$

Total energy	Potential energy	Kinetic energy	Virial theorem
-4204.788619	-8409.577640	4204.789030	-1.99999990

	Orbital	1s	2s	3s	4s	5s
	Energy	-758.04296	-109.06972	-20.13178	-3.15214	-0.23125
ζ_1	44249855.	.0000015	-.0000005	.0000002	-.0000001	.0000000
ζ_2	8746310.3	.0000085	-.0000027	.0000011	-.0000005	.0000001
ζ_3	2028606.5	.0000486	-.0000155	.0000066	-.0000026	.0000007
ζ_4	545088.33	.0002245	-.0000718	.0000305	-.0000122	.0000031
ζ_5	167170.19	.0008849	-.0002832	.0001200	-.0000479	.0000122
ζ_6	57561.853	.0030171	-.0009683	.0004109	-.0001642	.0000419
ζ_7	21873.986	.0090931	-.0029341	.0012445	-.0004970	.0001268
ζ_8	9018.3439	.0245754	-.0080465	.0034250	-.0013693	.0003492
ζ_9	3969.5313	.0597394	-.0201264	.0085833	-.0034311	.0008753
ζ_{10}	1838.5726	.1285653	-.0460546	.0198561	-.0079580	.0020305
ζ_{11}	885.02019	.2330823	-.0937072	.0409243	-.0164282	.0041940
ζ_{12}	438.23727	.3197515	-.1602736	.0726261	-.0293868	.0075083
ζ_{13}	221.42355	.2671114	-.1867242	.0887384	-.0361604	.0092558
ζ_{14}	113.44881	.0943713	-.0368149	.0202834	-.0086983	.0022336
ζ_{15}	58.673670	.0072561	.3602144	-.2383932	.1039403	-.0268570
ζ_{16}	30.529973	.0007929	.5523776	-.5071111	.2341286	-.0610951
ζ_{17}	15.946364	-.0003581	.2366401	-.2384243	.1187448	-.0314368
ζ_{18}	8.3481278	.0001718	.0243891	.5147349	-.3112507	.0848271
ζ_{19}	4.3760740	-.0001717	.0016346	.6874825	-.6939389	.2074164
ζ_{20}	2.2955552	.0001131	-.0000365	.1587117	-.1196354	.0261003
ζ_{21}	1.2046095	-.0000757	-.0001480	.0149665	.6455892	-.2351507
ζ_{22}	.63223283	.0000549	.0000105	-.0036040	.5921501	-.3086758
ζ_{23}	.33184700	-.0000362	-.0000460	.0039828	.1413959	-.1614460
ζ_{24}	.17418454	.0000228	.0000276	-.0025135	.0063364	.1190273
ζ_{25}	.09142912	-.0000126	-.0000164	.0014600	.0002565	.4441083
ζ_{26}	.04799105	.0000054	.0000072	-.0006386	.0000515	.4659533
ζ_{27}	.02519045	-.0000013	-.0000017	.0001552	-.0000222	.2006907

Table 43. Tc ^{6}S (27s, 20p, 17d; 27 ζ) (continued)

	Orbital	2p	3p	4p		3d	4d
	Energy	-100.40603	-16.69952	-2.04117		-10.44458	-0.54391
ζ_5	167170.19	.0000042	-.0000019	.0000007			
ζ_6	57561.853	.0000192	-.0000083	.0000031			
ζ_7	21873.986	.0001008	-.0000443	.0000166			
ζ_8	9018.3439	.0004275	-.0001862	.0000692			
ζ_9	3969.5313	.0016507	-.0007268	.0002723	ζ_9	.0000244	-.0000071
ζ_{10}	1838.5726	.0057359	-.0025210	.0009396	ζ_{10}	.0000851	-.0000256
ζ_{11}	885.02019	.0181704	-.0081198	.0030482	ζ_{11}	.0004488	-.0001312
ζ_{12}	438.23727	.0517077	-.0234580	.0087951	ζ_{12}	.0018942	-.0005646
ζ_{13}	221.42355	.1276078	-.0602763	.0228360	ζ_{13}	.0075198	-.0022230
ζ_{14}	113.44881	.2516655	-.1243751	.0473320	ζ_{14}	.0258484	-.0077342
ζ_{15}	58.673670	.3531821	-.1866844	.0724069	ζ_{15}	.0744203	-.0223515
ζ_{16}	30.529973	.2754985	-.1085955	.0377274	ζ_{16}	.1732270	-.0528864
ζ_{17}	15.946364	.0881225	.1891265	-.0965071	ζ_{17}	.2908457	-.0867526
ζ_{18}	8.3481278	.0088494	.4798881	-.2578637	ζ_{18}	.3427895	-.0966351
ζ_{19}	4.3760740	.0005017	.3840335	-.2313180	ζ_{19}	.2432213	-.0305823
ζ_{20}	2.2955552	.0001083	.0892406	.1679240	ζ_{20}	.0800432	.1397887
ζ_{21}	1.2046095	-.0001089	.0083928	.4774028	ζ_{21}	.0111692	.2987941
ζ_{22}	.63223283	.0000351	-.0007033	.4079208	ζ_{22}	.0002907	.3433065
ζ_{23}	.33184700	-.0000269	.0007687	.1331206	ζ_{23}	.0002963	.2681734
ζ_{24}	.17418454	.0000059	-.0002089	.0222263	ζ_{24}	-.0001199	.1286315
ζ_{25}	.09142912				ζ_{25}	.0000369	.0411067

Table 44. Ru ^{5}F (28s, 20p, 17d; 28 ζ)

		Symmetry species	S	P	D
		Number of basis functions	28	20	17
Nuclear charge	44	Number of closed shells	4	3	1
No. of electrons	44	Open-shell occupation	1	0	7

Coupling coefficients

$K_0^{ss} = -1.00000000$
$K_0^{dd} = -0.08571429 \quad K_2^{dd} = -0.01449396 \quad K_4^{dd} = -0.00283215$
$K_2^{sd} = -0.08571429$

Total energy	Potential energy	Kinetic energy	Virial theorem
-4441.539362	-8883.079750	4441.540380	-1.99999977

	Orbital	1s	2s	3s	4s	5s
	Energy	-795.51337	-115.15871	-21.41381	-3.25707	-0.22240
ζ_1	58766883.	.0000011	-.0000003	.0000001	-.0000001	.0000000
ζ_2	11888417.	.0000060	-.0000019	.0000008	-.0000003	.0000001
ζ_3	2795831.7	.0000342	-.0000110	.0000047	-.0000019	.0000004
ζ_4	755482.75	.0001579	-.0000506	.0000216	-.0000087	.0000021
ζ_5	231430.07	.0006270	-.0002009	.0000857	-.0000345	.0000082
ζ_6	79191.065	.0021669	-.0006961	.0002971	-.0001197	.0000285
ζ_7	29803.785	.0066540	-.0021463	.0009160	-.0003694	.0000881
ζ_8	12147.680	.0184055	-.0060062	.0025688	-.0010349	.0002468
ζ_9	5283.7615	.0460863	-.0153834	.0065952	-.0026627	.0006354
ζ_{10}	2419.8346	.1032918	-.0362422	.0156584	-.0063174	.0015071
ζ_{11}	1153.2329	.1991993	-.0768167	.0335904	-.0136196	.0032527
ζ_{12}	566.29590	.3029451	-.1405538	.0632252	-.0256805	.0061321
ζ_{13}	284.23647	.3031918	-.1908729	.0898827	-.0370312	.0088680
ζ_{14}	144.90730	.1454342	-.1097931	.0564798	-.0233294	.0055781
ζ_{15}	74.678121	.0190743	.2332631	-.1437147	.0614090	-.0147637
ζ_{16}	38.766172	.0012308	.5594836	-.4672297	.2162266	-.0527400
ζ_{17}	20.219429	-.0004760	.3473365	-.3931014	.1894019	-.0464201
ζ_{18}	10.577377	.0003331	.0534675	.3097257	-.1675169	.0415578
ζ_{19}	5.5432969	-.0003223	.0041016	.7615024	-.6804212	.1859782
ζ_{20}	2.9080944	.0002212	-.0009355	.2868672	-.3497322	.0964501
ζ_{21}	1.5264913	-.0001574	.0007021	.0184709	.5261109	-.1815356
ζ_{22}	.80150335	.0001155	-.0006661	.0032531	.6602136	-.2735516
ζ_{23}	.42089621	-.0000795	.0004264	-.0000566	.2501611	-.1940242
ζ_{24}	.22103926	.0000537	-.0002982	.0002438	.0152251	.0084288
ζ_{25}	.11608413	-.0000338	.0001869	-.0000685	.0049838	.2810709
ζ_{26}	.06096478	.0000187	-.0001067	.0000268	-.0034563	.5077329
ζ_{27}	.03201738	-.0000080	.0000434	-.0000092	.0005535	.3342789
ζ_{28}	.01681484	.0000019	-.0000110	.0000016	-.0003685	.0491711

Table 44. Ru ^{5}F (28s, 20p, 17d; 28 ζ) (continued)

	Orbital	2p	3p	4p		3d	4d
	Energy	-106.23931	-17.84868	-2.10120		-11.34327	-0.41274
ζ_5	231430.07	.0000026	-.0000012	.0000004			
ζ_6	79191.065	.0000121	-.0000053	.0000020			
ζ_7	29803.785	.0000648	-.0000287	.0000108			
ζ_8	12147.680	.0002806	-.0001230	.0000464			
ζ_9	5283.7615	.0011146	-.0004943	.0001865			
ζ_{10}	2419.8346	.0039734	-.0017560	.0006631	ζ_{10}	.0000840	-.0000245
ζ_{11}	1153.2329	.0130104	-.0058388	.0022077	ζ_{11}	.0002480	-.0000718
ζ_{12}	566.29590	.0383426	-.0174003	.0065999	ζ_{12}	.0013128	-.0003844
ζ_{13}	284.23647	.0999076	-.0470152	.0179274	ζ_{13}	.0051062	-.0014904
ζ_{14}	144.90730	.2126566	-.1042677	.0400877	ζ_{14}	.0188145	-.0055392
ζ_{15}	74.678121	.3366462	-.1768150	.0688746	ζ_{15}	.0568121	-.0168040
ζ_{16}	38.766172	.3203463	-.1564907	.0597978	ζ_{16}	.1429050	-.0429485
ζ_{17}	20.219429	.1364480	.0908925	-.0530052	ζ_{17}	.2639079	-.0785784
ζ_{18}	10.577377	.0188936	.4296196	-.2246097	ζ_{18}	.3444495	-.0979669
ζ_{19}	5.5432969	.0011885	.4565021	-.2839358	ζ_{19}	.2830851	-.0563333
ζ_{20}	2.9080944	-.0000021	.1494475	.0573053	ζ_{20}	.1123351	.0981840
ζ_{21}	1.5264913	.0000003	.0142483	.4355949	ζ_{21}	.0186542	.2619535
ζ_{22}	.80150335	-.0000482	.0007005	.4512916	ζ_{22}	.0012193	.3218389
ζ_{23}	.42089621	.0000057	.0004427	.1946791	ζ_{23}	.0004193	.2807788
ζ_{24}	.22103926	-.0000063	-.0000211	.0440392	ζ_{24}	.0000099	.1881859
ζ_{25}	.11608413				ζ_{25}	.0000926	.0848789
ζ_{26}	.06096478				ζ_{26}	-.0000029	.0222269

Table 45. Rh ^{4}F (28s, 20p, 17d; 28 ζ)

		Symmetry species	S	P	D
		Number of basis functions	28	20	17
Nuclear charge	45	Number of closed shells	4	3	1
No. of electrons	45	Open-shell occupation	1	0	8

Coupling coefficients

$K_0^{ss} = -1.00000000$
$K_0^{dd} = -0.05000000$ $K_2^{dd} = -0.00663265$ $K_4^{dd} = 0.00229592$
$K_2^{sd} = -0.05000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-4685.881574	-9371.764360	4685.882780	-1.99999974

	Orbital	1s	2s	3s	4s	5s
	Energy	-834.03936	-121.56355	-22.87953	-3.50383	-0.22159
ζ_1	62334830.	.0000010	-.0000003	.0000001	-.0000001	.0000000
ζ_2	12665107.	.0000059	-.0000019	.0000008	-.0000003	.0000001
ζ_3	2985726.8	.0000333	-.0000107	.0000046	-.0000019	.0000004
ζ_4	807485.99	.0001537	-.0000493	.0000212	-.0000086	.0000020
ζ_5	247279.61	.0006111	-.0001962	.0000842	-.0000343	.0000079
ζ_6	84521.390	.0021164	-.0006811	.0002923	-.0001192	.0000273
ζ_7	31762.718	.0065146	-.0021048	.0009035	-.0003688	.0000845
ζ_8	12926.401	.0180615	-.0059026	.0025392	-.0010354	.0002371
ζ_9	5615.1819	.0453226	-.0151473	.0065314	-.0026691	.0006115
ζ_{10}	2569.3288	.1018018	-.0357398	.0155301	-.0063422	.0014526
ζ_{11}	1224.0071	.1969095	-.0758988	.0333756	-.0136981	.0031408
ζ_{12}	601.13863	.3010501	-.1392835	.0629965	-.0259020	.0059383
ζ_{13}	301.92279	.3046797	-.1907671	.0902928	-.0376591	.0086581
ζ_{14}	154.09434	.1494253	-.1143031	.0590708	-.0247151	.0056757
ζ_{15}	79.530451	.0204969	.2227816	-.1377927	.0595948	-.0137584
ζ_{16}	41.358642	.0012500	.5564907	-.4643497	.2176666	-.0509759
ζ_{17}	21.614922	-.0004598	.3571837	-.4073977	.1994218	-.0469717
ζ_{18}	11.331963	.0003287	.0575316	.2942782	-.1610685	.0383534
ζ_{19}	5.9523232	-.0003221	.0042025	.7688637	-.6972411	.1832409
ζ_{20}	3.1300407	.0002217	-.0009410	.2949184	-.3564591	.0935606
ζ_{21}	1.6469432	-.0001581	.0007087	.0198143	.5310488	-.1762388
ζ_{22}	.86684956	.0001163	-.0006831	.0033471	.6588326	-.2572454
ζ_{23}	.45632420	-.0000802	.0004383	-.0000147	.2522354	-.1832355
ζ_{24}	.24023200	.0000542	-.0003076	.0002343	.0157902	-.0064555
ζ_{25}	.12647318	-.0000341	.0001935	-.0000573	.0055064	.2377341
ζ_{26}	.06658388	.0000189	-.0001093	.0000219	-.0030521	.4849209
ζ_{27}	.03505424	-.0000081	.0000451	-.0000058	.0008973	.3742474
ζ_{28}	.01845491	.0000019	-.0000113	.0000011	-.0003533	.0751576

Table 45. Rh ^{4}F (28s, 20p, 17d; 28 ζ) (continued)

	Orbital	2p	3p	4p		3d	4d
	Energy	-112.38609	-19.17951	-2.29109		-12.42121	-0.45015
ζ_5	247279.61	.0000025	-.0000011	.0000004			
ζ_6	84521.390	.0000117	-.0000052	.0000020			
ζ_7	31762.718	.0000630	-.0000281	.0000108			
ζ_8	12926.401	.0002738	-.0001209	.0000463			
ζ_9	5615.1819	.0010900	-.0004870	.0001867			
ζ_{10}	2569.3288	.0038923	-.0017328	.0006647	ζ_{10}	.0000832	-.0000253
ζ_{11}	1224.0071	.0127589	-.0057680	.0022161	ζ_{11}	.0002460	-.0000740
ζ_{12}	601.13863	.0376388	-.0172041	.0066294	ζ_{12}	.0013028	-.0003969
ζ_{13}	301.92279	.0982234	-.0465519	.0180384	ζ_{13}	.0050639	-.0015359
ζ_{14}	154.09434	.2098082	-.1036015	.0404757	ζ_{14}	.0186771	-.0057199
ζ_{15}	79.530451	.3343282	-.1768662	.0700400	ζ_{15}	.0564947	-.0173757
ζ_{16}	41.358642	.3224567	-.1599179	.0622170	ζ_{16}	.1424480	-.0445593
ζ_{17}	21.614922	.1406630	.0839151	-.0509090	ζ_{17}	.2640208	-.0818137
ζ_{18}	11.331963	.0200773	.4278999	-.2288733	ζ_{18}	.3458394	-.1024369
ζ_{19}	5.9523232	.0012223	.4608614	-.2920506	ζ_{19}	.2827608	-.0567657
ζ_{20}	3.1300407	-.0000214	.1514950	.0606586	ζ_{20}	.1101421	.1075170
ζ_{21}	1.6469432	.0000005	.0147360	.4404193	ζ_{21}	.0179610	.2722255
ζ_{22}	.86684956	-.0000564	.0007363	.4490276	ζ_{22}	.0012111	.3237756
ζ_{23}	.45632420	.0000072	.0004907	.1924538	ζ_{23}	.0005149	.2748434
ζ_{24}	.24023200	-.0000073	-.0000168	.0434847	ζ_{24}	.0000427	.1791578
ζ_{25}	.12647318				ζ_{25}	.0001191	.0783749
ζ_{26}	.06658388				ζ_{26}	-.0000004	.0200687

Table 45. Rh ^{4}F (28s, 20p, 17d; 28 ζ)

		Symmetry species	S	P	D
		Number of basis functions	28	20	17
Nuclear charge	45	Number of closed shells	4	3	1
No. of electrons	45	Open-shell occupation	1	0	8

Coupling coefficients

$K_0^{ss} = -1.00000000$
$K_0^{dd} = -0.05000000$ $K_2^{dd} = -0.00663265$ $K_4^{dd} = 0.00229592$
$K_2^{sd} = -0.05000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-4685.881602	-9371.763110	4685.881510	-2.00000002

	Orbital	1s	2s	3s	4s	5s
	Energy	-834.03943	-121.56362	-22.87959	-3.50387	-0.22160
ζ_1	85480152.	.0000008	-.0000003	.0000001	.0000000	.0000000
ζ_2	13162129.	.0000062	-.0000020	.0000008	-.0000003	.0000001
ζ_3	2952111.5	.0000339	-.0000109	.0000047	-.0000019	.0000004
ζ_4	801195.70	.0001540	-.0000494	.0000212	-.0000086	.0000020
ζ_5	247279.61	.0006095	-.0001957	.0000839	-.0000343	.0000078
ζ_6	84521.390	.0021179	-.0006815	.0002925	-.0001192	.0000273
ζ_7	31762.718	.0065129	-.0021045	.0009036	-.0003688	.0000845
ζ_8	12926.401	.0180636	-.0059024	.0025385	-.0010350	.0002371
ζ_9	5615.1819	.0453199	-.0151493	.0065341	-.0026706	.0006118
ζ_{10}	2569.3288	.1018054	-.0357322	.0155211	-.0063374	.0014519
ζ_{11}	1224.0071	.1969044	-.0759217	.0334012	-.0137117	.0031432
ζ_{12}	601.13863	.3010583	-.1392206	.0629281	-.0258657	.0059323
ζ_{13}	301.92279	.3046645	-.1909367	.0904706	-.0377526	.0086749
ζ_{14}	154.09434	.1494628	-.1137875	.0585760	-.0244607	.0056289
ζ_{15}	79.419473	.0205007	.2222638	-.1370241	.0591599	-.0136840
ζ_{16}	41.420047	.0012022	.5548477	-.4637500	.2175713	-.0508994
ζ_{17}	21.648176	-.0004322	.3589853	-.4068181	.1986363	-.0468994
ζ_{18}	11.331963	.0003119	.0573156	.2884886	-.1565388	.0374758
ζ_{19}	5.9884769	-.0003084	.0044971	.7672928	-.6946387	.1819521
ζ_{20}	3.1306967	.0002085	-.0011489	.3034197	-.3667056	.0974992
ζ_{21}	1.6518684	-.0001471	.0008680	.0152434	.5351721	-.1794502
ζ_{22}	.86684956	.0001050	-.0007802	.0064212	.6591295	-.2534363
ζ_{23}	.45437838	-.0000683	.0004789	-.0020064	.2545137	-.1935519
ζ_{24}	.22582157	.0000469	-.0003417	.0016287	.0137456	.0236281
ζ_{25}	.11822694	-.0000369	.0002692	-.0012000	.0058826	.2044452
ζ_{26}	.07073925	.0000216	-.0001597	.0006984	-.0037802	.4571231
ζ_{27}	.03507515	-.0000065	.0000463	-.0002074	.0007632	.4348550
ζ_{28}	.01639887	.0000013	-.0000098	.0000420	-.0002767	.0534036

Table 45. Rh ^{4}F (28s, 20p, 17d; 28 ζ) (continued)

	Orbital	2p	3p	4p		3d	4d
	Energy	-112.38616	-19.17957	-2.29113		-12.42126	-0.45017
ζ_5	247279.61	.0000025	-.0000011	.0000004			
ζ_6	84521.390	.0000118	-.0000052	.0000020			
ζ_7	31762.718	.0000627	-.0000279	.0000107			
ζ_8	12926.401	.0002747	-.0001217	.0000466			
ζ_9	5615.1819	.0010869	-.0004846	.0001858			
ζ_{10}	2569.3288	.0039016	-.0017402	.0006674	ζ_{10}	.0000832	-.0000255
ζ_{11}	1224.0071	.0127325	-.0057471	.0022086	ζ_{11}	.0002459	-.0000732
ζ_{12}	601.13863	.0377104	-.0172602	.0066497	ζ_{12}	.0013035	-.0003995
ζ_{13}	301.92279	.0980292	-.0464033	.0179840	ζ_{13}	.0050588	-.0015279
ζ_{14}	154.09434	.2104174	-.1040352	.0406375	ζ_{14}	.0187169	-.0057482
ζ_{15}	79.419473	.3341356	-.1764981	.0699137	ζ_{15}	.0565816	-.0173643
ζ_{16}	41.420047	.3210487	-.1599084	.0621928	ζ_{16}	.1414529	-.0443367
ζ_{17}	21.648176	.1420757	.0842046	-.0509456	ζ_{17}	.2650357	-.0819361
ζ_{18}	11.331963	.0195384	.4253382	-.2278051	ζ_{18}	.3443188	-.1024453
ζ_{19}	5.9884769	.0016589	.4594604	-.2899074	ζ_{19}	.2819121	-.0560053
ζ_{20}	3.1306967	-.0003248	.1567906	.0543005	ζ_{20}	.1134257	.1053206
ζ_{21}	1.6518684	.0002051	.0120295	.4441309	ζ_{21}	.0161280	.2734848
ζ_{22}	.86684956	-.0001740	.0022911	.4468706	ζ_{22}	.0024868	.3227495
ζ_{23}	.45437838	.0000581	-.0001987	.1995705	ζ_{23}	-.0002727	.2851483
ζ_{24}	.22582157	-.0000195	.0001590	.0382102	ζ_{24}	.0005332	.1885214
ζ_{25}	.11822694				ζ_{25}	-.0001792	.0569647
ζ_{26}	.07073925				ζ_{26}	.0001012	.0228988

Table 46. Pd ^{1}S (25s, 20p, 17d; 27 ζ)

		Symmetry species	S	P	D
		Number of basis functions	25	20	17
Nuclear charge	46	Number of closed shells	4	3	2
No. of electrons	46	Open-shell occupation	0	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-4937.920897	-9875.843750	4937.922850	-1.99999961

	Orbital	1s	2s	3s	4s
	Energy	-873.31575	-127.96640	-24.20895	-3.58719
ζ_1	130626290.	.0000004	-.0000001	.0000001	.0000000
ζ_2	27498757.	.0000023	-.0000007	.0000003	-.0000001
ζ_3	6605763.6	.0000130	-.0000042	.0000018	-.0000007
ζ_4	1794880.2	.0000599	-.0000193	.0000083	-.0000034
ζ_5	546036.04	.0002426	-.0000780	.0000337	-.0000138
ζ_6	183890.14	.0008639	-.0002779	.0001198	-.0000492
ζ_7	67732.003	.0027564	-.0008894	.0003840	-.0001576
ζ_8	26948.965	.0079789	-.0025865	.0011161	-.0004583
ζ_9	11441.836	.0211532	-.0069486	.0030084	-.0012353
ζ_{10}	5124.1663	.0513065	-.0172774	.0074919	-.0030798
ζ_{11}	2395.1302	.1119937	-.0398178	.0174366	-.0071746
ζ_{12}	1157.6121	.2101580	-.0826886	.0366281	-.0151228
ζ_{13}	573.94929	.3082209	-.1476448	.0675815	-.0280375
ζ_{14}	290.00944	.2912298	-.1910846	.0915080	-.0383926
ζ_{15}	148.55907	.1272321	-.0880467	.0469380	-.0200151
ζ_{16}	76.835850	.0141074	.2778918	-.1794038	.0794432
ζ_{17}	40.001056	.0010827	.5637708	-.4946092	.2346103
ζ_{18}	20.914449	-.0004832	.3092472	-.3538355	.1789078
ζ_{19}	10.964768	.0003007	.0408114	.4101825	-.2451742
ζ_{20}	5.7578601	-.0002769	.0029096	.7522685	-.7453603
ζ_{21}	3.0263932	.0001789	-.0006684	.2174592	-.2015844
ζ_{22}	1.5914853	-.0001103	.0003153	.0164701	.6104781
ζ_{23}	.83711076	.0000639	-.0002970	-.0000045	.6049453
ζ_{24}	.44035951	-.0000269	.0001002	.0013197	.1888941
ζ_{25}	.23165830	.0000065	-.0000276	-.0001845	.0200619
ζ_{26}	.12186891				
ζ_{27}	.06411193				

Table 46. Pd ^{1}S (25s, 20p, 17d; 27 ζ) (continued)

	Orbital	2p	3p	4p		3d	4d
	Energy	-118.53093	-20.37413	-2.32997		-13.36328	-0.33591
ζ_6	183890.14	.0000045	-.0000020	.0000008			
ζ_7	67732.003	.0000171	-.0000075	.0000029			
ζ_8	26948.965	.0000867	-.0000390	.0000151			
ζ_9	11441.836	.0003507	-.0001559	.0000600			
ζ_{10}	5124.1663	.0013379	-.0006027	.0002336			
ζ_{11}	2395.1302	.0046270	-.0020752	.0008005	ζ_{11}	.0001091	-.0000328
ζ_{12}	1157.6121	.0148096	-.0067571	.0026234	ζ_{12}	.0003039	-.0000899
ζ_{13}	573.94929	.0428540	-.0197856	.0076759	ζ_{13}	.0015989	-.0004824
ζ_{14}	290.00944	.1093145	-.0524731	.0205537	ζ_{14}	.0061096	-.0018284
ζ_{15}	148.55907	.2265426	-.1134880	.0446915	ζ_{15}	.0220334	-.0066786
ζ_{16}	76.835850	.3441390	-.1849796	.0742041	ζ_{16}	.0653352	-.0198748
ζ_{17}	40.001056	.3054585	-.1431677	.0546347	ζ_{17}	.1595501	-.0494438
ζ_{18}	20.914449	.1176708	.1310804	-.0736690	ζ_{18}	.2827238	-.0861381
ζ_{19}	10.964768	.0141343	.4659159	-.2593969	ζ_{19}	.3506506	-.1014455
ζ_{20}	5.7578601	.0008058	.4272439	-.2708935	ζ_{20}	.2579345	-.0354726
ζ_{21}	3.0263932	-.0000280	.1122789	.1438111	ζ_{21}	.0849255	.1427166
ζ_{22}	1.5914853	-.0000433	.0108566	.4676757	ζ_{22}	.0117472	.2839251
ζ_{23}	.83711076	-.0000307	-.0002106	.4099044	ζ_{23}	.0003153	.3082560
ζ_{24}	.44035951	-.0000049	.0008362	.1588630	ζ_{24}	.0004045	.2507541
ζ_{25}	.23165830	-.0000050	-.0000812	.0354446	ζ_{25}	-.0001862	.1740303
ζ_{26}	.12186891				ζ_{26}	.0000991	.0863159
ζ_{27}	.06411193				ζ_{27}	-.0000292	.0335991

Table 47. Ag ^{2}S (28s, 20p, 17d; 28 ζ)

Nuclear charge	47
No. of electrons	47

Symmetry species	S	P	D
Number of basis functions	28	20	17
Number of closed shells	4	3	2
Open-shell occupation	1	0	0

Coupling coefficients
$K_0^{ss} = -1.00000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-5197.698318	-10395.39660	5197.698240	-2.00000002

	Orbital	1s	2s	3s	4s	5s
	Energy	-913.83552	-134.87837	-25.91778	-4.00146	-0.21996
ζ_1	45797651.	.0000017	-.0000006	.0000002	-.0000001	.0000000
ζ_2	9172008.3	.0000099	-.0000032	.0000014	-.0000006	.0000001
ζ_3	2143663.3	.0000565	-.0000182	.0000079	-.0000033	.0000007
ζ_4	577660.58	.0002609	-.0000840	.0000364	-.0000152	.0000032
ζ_5	176988.26	.0010321	-.0003327	.0001442	-.0000600	.0000126
ζ_6	60714.974	.0035414	-.0011449	.0004969	-.0002070	.0000435
ζ_7	22947.634	.0107438	-.0034970	.0015177	-.0006312	.0001325
ζ_8	9403.8165	.0291444	-.0096407	.0041982	-.0017514	.0003680
ζ_9	4115.0385	.0706169	-.0241707	.0105604	-.0043949	.0009227
ζ_{10}	1896.4270	.1494434	-.0548762	.0242586	-.0101585	.0021361
ζ_{11}	909.41523	.2600300	-.1094158	.0492040	-.0205673	.0043204
ζ_{12}	449.24291	.3271112	-.1767507	.0828774	-.0351915	.0074185
ζ_{13}	226.76205	.2318372	-.1762708	.0875687	-.0370698	.0077941
ζ_{14}	116.22110	.0609616	.0435294	-.0242656	.0095933	-.0019699
ζ_{15}	60.194058	.0030786	.4599141	-.3388670	.1592355	-.0341438
ζ_{16}	31.394982	.0002257	.5049084	-.5247391	.2555296	-.0548563
ζ_{17}	16.448596	-.0000324	.1525730	-.0557055	.0416781	-.0100939
ζ_{18}	8.6421072	-.0000911	.0113026	.7119539	-.5512502	.1295754
ζ_{19}	4.5482183	.0000438	-.0002119	.5403009	-.6559295	.1615211
ζ_{20}	2.3959603	-.0000370	.0006277	.0591843	.2662093	-.0857054
ζ_{21}	1.2628229	.0000326	-.0007365	.0152309	.7095539	-.2252267
ζ_{22}	0.6657608	-.0000220	.0004735	-.0071642	.4177301	-.1981499
ζ_{23}	.35103158	.0000159	-.0003632	.0059871	.0564584	-.0817060
ζ_{24}	.18509546	-.0000107	.0002472	-.0040172	.0097766	.0855865
ζ_{25}	.09760073	.0000068	-.0001574	.0025816	-.0043596	.3449197
ζ_{26}	.05146508	-.0000037	.0000877	-.0014462	.0029112	.4823292
ζ_{27}	.02713768	.0000016	-.0000374	.0006189	-.0011485	.2412251
ζ_{28}	.01430978	-.0000004	.0000090	-.0001488	.0003069	.0208421

Table 47. Ag ^{2}S (28s, 20p, 17d; 28 ζ) (continued)

	Orbital	2p	3p	4p		3d	4d
	Energy	-125.18155	-21.94539	-2.67678		-14.67816	-0.53737
ζ_5	176988.26	.0000053	-.0000024	.0000009			
ζ_6	60714.974	.0000245	-.0000110	.0000043			
ζ_7	22947.634	.0001288	-.0000579	.0000229			
ζ_8	9403.8165	.0005541	-.0002496	.0000978			
ζ_9	4115.0385	.0021475	-.0009701	.0003834	ζ_9	.0000372	-.0000118
ζ_{10}	1896.4270	.0074946	-.0034081	.0013389	ζ_{10}	.0001276	-.0000412
ζ_{11}	909.41523	.0235374	-.0108379	.0042944	ζ_{11}	.0006918	-.0002211
ζ_{12}	449.24291	.0659093	-.0311075	.0123132	ζ_{12}	.0028548	-.0009217
ζ_{13}	226.76205	.1559608	-.0766311	.0307188	ζ_{13}	.0112580	-.0036317
ζ_{14}	116.22110	.2876434	-.1496765	.0603499	ζ_{14}	.0369746	-.0120452
ζ_{15}	60.194058	.3555591	-.1933684	.0794269	ζ_{15}	.1023748	-.0337080
ζ_{16}	31.394982	.2254470	-.0473942	.0096945	ζ_{16}	.2178556	-.0724286
ζ_{17}	16.448596	.0534365	.3016883	-.1623641	ζ_{17}	.3300186	-.1059363
ζ_{18}	8.6421072	.0038188	.5162914	-.3225884	ζ_{18}	.3302984	-.0919245
ζ_{19}	4.5482183	.0000537	.2747701	-.1152142	ζ_{19}	.1697859	.0484010
ζ_{20}	2.3959603	.0000728	.0374707	.3544407	ζ_{20}	.0355723	.2429012
ζ_{21}	1.2628229	-.0001482	.0046719	.4848255	ζ_{21}	.0033379	.3278637
ζ_{22}	0.6657608	.0000491	-.0006880	.2932946	ζ_{22}	-.0000132	.2945991
ζ_{23}	.35103158	-.0000355	.0006820	.0695498	ζ_{23}	.0001789	.2035762
ζ_{24}	.18509546	.0000072	-.0001371	.0099651	ζ_{24}	-.0000767	.0955447
ζ_{25}	.09760073				ζ_{25}	.0000234	.0323047

Table 48. Cd ^{1}S (28s, 20p, 17d; 28 ζ)

		Symmetry species	S	P	D
		Number of basis functions	28	20	17
Nuclear charge	48	Number of closed shells	5	3	2
No. of electrons	48	Open-shell occupation	0	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-5465.132996	-10930.26550	5465.132530	-2.00000008

	Orbital	1s	2s	3s	4s	5s
	Energy	-955.31531	-142.00680	-27.70859	-4.45051	-0.26484
ζ_1	52606084.	.0000015	-.0000005	.0000002	-.0000001	.0000000
ζ_2	10583073.	.0000087	-.0000028	.0000012	-.0000005	.0000001
ζ_3	2479281.7	.0000496	-.0000160	.0000070	-.0000029	.0000007
ζ_4	668574.92	.0002291	-.0000739	.0000322	-.0000136	.0000032
ζ_5	204765.18	.0009077	-.0002930	.0001276	-.0000539	.0000128
ζ_6	70179.584	.0031210	-.0010103	.0004407	-.0001863	.0000443
ζ_7	26500.195	.0094922	-.0030908	.0013478	-.0005690	.0001352
ζ_8	10853.996	.0258389	-.0085405	.0037375	-.0015817	.0003761
ζ_9	4750.5708	.0629991	-.0214682	.0094171	-.0039783	.0009454
ζ_{10}	2191.7188	.1350644	-.0490806	.0217787	-.0092479	.0022006
ζ_{11}	1053.1878	.2415483	-.0992136	.0446611	-.0189476	.0045052
ζ_{12}	521.82543	.3220816	-.1664195	.0779314	-.0335018	.0079902
ζ_{13}	264.41160	.2564031	-.1855168	.0914230	-.0393282	.0093656
ζ_{14}	136.13576	.0840225	-.0155531	.0093593	-.0049329	.0012372
ζ_{15}	70.871140	.0058032	.3883261	-.2736221	.1289797	-.0312743
ζ_{16}	37.170532	.0006082	.5407943	-.5282942	.2598298	-.0631872
ζ_{17}	19.589964	-.0002679	.2154672	-.2047542	.1192697	-.0304357
ζ_{18}	10.356004	.0000955	.0202118	.6038657	-.4361806	.1148240
ζ_{19}	5.4846649	-.0001075	.0009419	.6538347	-.7520640	.2110155
ζ_{20}	2.9078269	.0000707	.0000343	.1127128	.0732550	-.0373296
ζ_{21}	1.5425458	-.0000452	-.0002916	.0181933	.7060740	-.2499487
ζ_{22}	0.8185317	.0000341	.0001236	-.0072077	.5118930	-.2624646
ζ_{23}	.43440308	-.0000231	-.0001243	.0065445	.0940982	-.1181102
ζ_{24}	.23055552	.0000156	.0000844	-.0044330	.0089579	.1237467
ζ_{25}	.12236787	-.0000098	-.0000548	.0028779	-.0030258	.3759991
ζ_{26}	.06494744	.0000054	.0000307	-.0016130	.0019518	.4640079
ζ_{27}	.03447127	-.0000023	-.0000131	.0006918	-.0008779	.2279251
ζ_{28}	.01829585	.0000005	.0000031	-.0001651	.0002154	.0224624

Table 48. Cd ^{1}S (28s, 20p, 17d; 28 ζ) (continued)

	Orbital	2p	3p	4p		3d	4d
	Energy	-132.04700	-23.59721	-3.05348		-16.07195	-0.76364
ζ_5	204765.18	.0000045	-.0000020	.0000008			
ζ_6	70179.584	.0000205	-.0000092	.0000037			
ζ_7	26500.195	.0001084	-.0000492	.0000198			
ζ_8	10853.996	.0004660	-.0002107	.0000840			
ζ_9	4750.5708	.0018110	-.0008244	.0003323	ζ_9	.0000301	-.0000101
ζ_{10}	2191.7188	.0063215	-.0028846	.0011535	ζ_{10}	.0001043	-.0000360
ζ_{11}	1053.1878	.0199576	-.0092407	.0037319	ζ_{11}	.0005591	-.0001883
ζ_{12}	521.82543	.0563498	-.0266065	.0107161	ζ_{12}	.0023214	-.0007963
ζ_{13}	264.41160	.1365520	-.0671332	.0274059	ζ_{13}	.0091691	-.0031252
ζ_{14}	136.13576	.2626323	-.1359018	.0556954	ζ_{14}	.0307550	-.0106202
ζ_{15}	70.871140	.3532275	-.1942415	.0814401	ζ_{15}	.0870518	-.0302707
ζ_{16}	37.170532	.2595455	-.0936735	.0322408	ζ_{16}	.1945633	-.0687467
ζ_{17}	19.589964	.0772918	.2287414	-.1267811	ζ_{17}	.3129648	-.1073688
ζ_{18}	10.356004	.0068350	.5085320	-.3147432	ζ_{18}	.3423723	-.1071424
ζ_{19}	5.4846649	.0002888	.3421075	-.1968758	ζ_{19}	.2029136	.0160342
ζ_{20}	2.9078269	.0000082	.0623060	.2811603	ζ_{20}	.0506309	.2249031
ζ_{21}	1.5425458	-.0001161	.0071248	.4973532	ζ_{21}	.0055716	.3365290
ζ_{22}	0.8185317	.0000197	-.0009259	.3446941	ζ_{22}	-.0000836	.3132757
ζ_{23}	.43440308	-.0000250	.0009237	.0916981	ζ_{23}	.0002895	.2085887
ζ_{24}	.23055552	.0000044	-.0002145	.0142013	ζ_{24}	-.0001306	.0893097
ζ_{25}	.12236787				ζ_{25}	.0000388	.0248162

Table 49. In ^{2}P (28s, 23p, 17d; 28 ζ)

		Symmetry species	S	P	D
		Number of basis functions	28	23	17
Nuclear charge	49	Number of closed shells	5	3	2
No. of electrons	49	Open-shell occupation	0	1	0

Coupling coefficients

$K_0^{pp} = -1.66666667$ $K_2^{pp} = 0.13333333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-5740.169018	-11480.33970	5740.170660	-1.99999972

	Orbital	1s	2s	3s	4s	5s
	Energy	-997.80030	-149.39532	-29.62455	-4.97661	-0.37262
ζ_1	87470639.	.0000008	-.0000003	.0000001	-.0000001	.0000000
ζ_2	18006198.	.0000047	-.0000015	.0000007	-.0000003	.0000001
ζ_3	4262079.9	.0000265	-.0000085	.0000037	-.0000016	.0000004
ζ_4	1148864.2	.0001232	-.0000398	.0000174	-.0000075	.0000020
ζ_5	348743.03	.0004973	-.0001607	.0000704	-.0000302	.0000081
ζ_6	117744.77	.0017559	-.0005685	.0002490	-.0001066	.0000287
ζ_7	43636.064	.0055182	-.0017930	.0007856	-.0003368	.0000908
ζ_8	17513.635	.0156158	-.0051247	.0022495	-.0009633	.0002596
ζ_9	7513.1800	.0399823	-.0133921	.0058919	-.0025290	.0006819
ζ_{10}	3402.7327	.0917115	-.0321183	.0142292	-.0061021	.0016445
ζ_{11}	1608.9689	.1820745	-.0695012	.0311445	-.0134257	.0036232
ζ_{12}	786.62700	.2895190	-.1307139	.0601133	-.0259495	.0070000
ζ_{13}	394.40848	.3143835	-.1890314	.0908268	-.0397888	.0107710
ζ_{14}	201.46156	.1749643	-.1393574	.0726218	-.0319266	.0086281
ζ_{15}	104.28583	.0304661	.1620977	-.1004190	.0452892	-.0122829
ζ_{16}	54.487318	.0014782	.5344292	-.4370766	.2151251	-.0594501
ζ_{17}	28.648280	-.0003283	.4113200	-.4740164	.2451946	-.0681826
ζ_{18}	15.124869	.0002779	.0839232	.1893398	-.1041859	.0286611
ζ_{19}	8.0059708	-.0003024	.0052227	.7908371	-.7404475	.2322373
ζ_{20}	4.2444232	.0002093	-.0008388	.3571797	-.4436165	.1372310
ζ_{21}	2.2522420	-.0001517	.0006897	.0284659	.5181048	-.2037730
ζ_{22}	1.1957015	.0001134	-.0007324	.0053648	.7000010	-.3331963
ζ_{23}	.63494496	-.0000786	.0004753	-.0010035	.2651399	-.2547751
ζ_{24}	.33720751	.0000533	-.0003376	.0009592	.0105744	.0627143
ζ_{25}	.17909250	-.0000336	.0002150	-.0005413	.0064658	.3868912
ζ_{26}	.09511826	.0000185	-.0001193	.0002860	-.0032386	.5015695
ζ_{27}	.05051868	-.0000079	.0000510	-.0001218	.0014668	.2569303
ζ_{28}	.02683121	.0000019	-.0000121	.0000283	-.0003439	.0337814

Table 49. In ^{2}P (28s, 23p, 17d; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-139.17180	-25.37417	-3.50713	-0.19725
ζ_6	117744.77	.0000124	-.0000056	.0000023	-.0000005
ζ_7	43636.064	.0000460	-.0000211	.0000086	-.0000017
ζ_8	17513.635	.0002282	-.0001034	.0000422	-.0000084
ζ_9	7513.1800	.0009039	-.0004142	.0001694	-.0000337
ζ_{10}	3402.7327	.0033172	-.0015148	.0006187	-.0001230
ζ_{11}	1608.9689	.0110236	-.0051072	.0020930	-.0004169
ζ_{12}	786.62700	.0330446	-.0154685	.0063484	-.0012633
ζ_{13}	394.40848	.0877606	-.0425259	.0175756	-.0035042
ζ_{14}	201.46156	.1927634	-.0972725	.0404965	-.0080745
ζ_{15}	104.28583	.3208164	-.1733310	.0732902	-.0146610
ζ_{16}	54.487318	.3350189	-.1771683	.0742642	-.0148037
ζ_{17}	28.648280	.1663408	.0408591	-.0335597	.0071324
ζ_{18}	15.124869	.0282575	.4045281	-.2355659	.0493118
ζ_{19}	8.0059708	.0015719	.4863024	-.3298621	.0702524
ζ_{20}	4.2444232	-.0000758	.1753433	.0391625	-.0160917
ζ_{21}	2.2522420	.0000118	.0191480	.4585329	-.1180442
ζ_{22}	1.1957015	-.0001082	.0009011	.4594474	-.1264141
ζ_{23}	.63494496	.0000422	.0008289	.1932101	-.0641567
ζ_{24}	.33720751	-.0000382	-.0003939	.0261601	.0822649
ζ_{25}	.17909250	.0000234	.0002847	.0037363	.2378889
ζ_{26}	.09511826	-.0000134	-.0001757	-.0002970	.3855723
ζ_{27}	.05051868	.0000061	.0000785	.0004485	.3074536
ζ_{28}	.02683121	-.0000016	-.0000215	-.0000715	.1513926

	Orbital	3d	4d
	Energy	-17.58945	-1.06306
ζ_9	7513.1800	.0000118	-.0000041
ζ_{10}	3402.7327	.0000472	-.0000172
ζ_{11}	1608.9689	.0002475	-.0000872
ζ_{12}	786.62700	.0011177	-.0004036
ζ_{13}	394.40848	.0045637	-.0016299
ζ_{14}	201.46156	.0169150	-.0061291
ζ_{15}	104.28583	.0522522	-.0189697
ζ_{16}	54.487318	.1346457	-.0499140
ζ_{17}	28.648280	.2576915	-.0947992
ζ_{18}	15.124869	.3489079	-.1233833
ζ_{19}	8.0059708	.2900064	-.0664164
ζ_{20}	4.2444232	.1119824	.1344326
ζ_{21}	2.2522420	.0177073	.3183676
ζ_{22}	1.1957015	.0007758	.3500753
ζ_{23}	.63494496	.0002784	.2604504
ζ_{24}	.33720751	-.0001001	.1141768
ζ_{25}	.17909250	.0000266	.0354249

Table 50. Sn ^{3}P (28s, 23p, 17d; 28 ζ)

		Symmetry species	S	P	D
		Number of basis functions	28	23	17
Nuclear charge	50	Number of closed shells	5	3	2
No. of electrons	50	Open-shell occupation	0	2	0

Coupling coefficients

$K_0^{pp} = -0.66666667$ $K_2^{pp} = -0.06666667$

Total energy	Potential energy	Kinetic energy	Virial theorem
-6022.931572	-12045.86360	6022.931980	-1.99999994

	Orbital	1s	2s	3s	4s	5s
	Energy	-1041.22326	-156.97752	-31.59892	-5.51245	-0.47641
ζ_1	92533822.	.0000008	-.0000003	.0000001	-.0000001	.0000000
ζ_2	19290575.	.0000045	-.0000014	.0000006	-.0000003	.0000001
ζ_3	4600810.6	.0000252	-.0000082	.0000036	-.0000016	.0000005
ζ_4	1244348.4	.0001171	-.0000379	.0000167	-.0000072	.0000021
ζ_5	377768.80	.0004739	-.0001534	.0000675	-.0000293	.0000086
ζ_6	127273.26	.0016810	-.0005449	.0002398	-.0001041	.0000304
ζ_7	47008.759	.0053123	-.0017284	.0007608	-.0003307	.0000967
ζ_8	18797.752	.0151146	-.0049650	.0021889	-.0009502	.0002778
ζ_9	8037.8160	.0388788	-.0130307	.0057597	-.0025064	.0007333
ζ_{10}	3632.1184	.0895140	-.0313340	.0139396	-.0060593	.0017714
ζ_{11}	1715.8784	.1783874	-.0679567	.0305884	-.0133690	.0039150
ζ_{12}	839.41314	.2855015	-.1281329	.0591230	-.0258652	.0075686
ζ_{13}	421.78083	.3149637	-.1872693	.0902944	-.0401098	.0117857
ζ_{14}	216.21547	.1819191	-.1452333	.0756350	-.0336694	.0098647
ζ_{15}	112.46515	.0344837	.1396026	-.0860205	.0390724	-.0114641
ζ_{16}	59.107083	.0016394	.5178643	-.4184153	.2086146	-.0626450
ζ_{17}	31.286316	-.0002426	.4312148	-.4917132	.2569070	-.0774611
ζ_{18}	16.639226	.0002338	.0998578	.1218954	-.0621171	.0176433
ζ_{19}	8.8764615	-.0002769	.0061973	.7797851	-.7191412	.2453150
ζ_{20}	4.7442364	.0001898	-.0005495	.4077346	-.5217769	.1781193
ζ_{21}	2.5384839	-.0001392	.0005386	.0377599	.4563628	-.1955612
ζ_{22}	1.3590930	.0001056	-.0006539	.0075472	.7326185	-.3791423
ζ_{23}	.72788210	-.0000732	.0004160	-.0022050	.3023733	-.3086039
ζ_{24}	.38988551	.0000498	-.0003003	.0018784	.0137975	.0852521
ζ_{25}	.20885248	-.0000314	.0001926	-.0011554	.0075528	.4357294
ζ_{26}	.11187973	.0000172	-.0001063	.0006214	-.0036308	.5053516
ζ_{27}	.05993295	-.0000073	.0000453	-.0002677	.0017037	.2257874
ζ_{28}	.03210556	.0000017	-.0000107	.0000623	-.0003906	.0247307

Table 50. Sn ^{3}P (28s, 23p, 17d; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-146.48920	-27.20898	-3.96900	-0.26502
ζ_6	127273.26	.0000116	-.0000053	.0000022	-.0000005
ζ_7	47008.759	.0000437	-.0000201	.0000084	-.0000020
ζ_8	18797.752	.0002179	-.0000994	.0000413	-.0000096
ζ_9	8037.8160	.0008682	-.0003998	.0001664	-.0000388
ζ_{10}	3632.1184	.0031972	-.0014689	.0006114	-.0001425
ζ_{11}	1715.8784	.0106354	-.0049525	.0020655	-.0004817
ζ_{12}	839.41314	.0318710	-.0150021	.0062728	-.0014632
ζ_{13}	421.78083	.0845776	-.0411651	.0173158	-.0040433
ζ_{14}	216.21547	.1862849	-.0944181	.0400464	-.0093610
ζ_{15}	112.46515	.3131835	-.1697199	.0730231	-.0171085
ζ_{16}	59.107083	.3367921	-.1813733	.0778425	-.0182207
ζ_{17}	31.286316	.1775959	.0195369	-.0235693	.0060613
ζ_{18}	16.639226	.0335449	.3797955	-.2249134	.0552266
ζ_{19}	8.8764615	.0019133	.4958164	-.3425055	.0861578
ζ_{20}	4.7442364	-.0000220	.1992618	-.0009856	-.0086890
ζ_{21}	2.5384839	-.0000148	.0239482	.4425359	-.1351730
ζ_{22}	1.3590930	-.0001019	.0016323	.4790921	-.1588634
ζ_{23}	.72788210	.0000347	.0005262	.2094990	-.0822093
ζ_{24}	.38988551	-.0000341	-.0001620	.0284417	.1062503
ζ_{25}	.20885248	.0000210	.0001254	.0041378	.3016711
ζ_{26}	.11187973	-.0000119	-.0000855	-.0004278	.4030544
ζ_{27}	.05993295	.0000055	.0000362	.0005291	.2715331
ζ_{28}	.03210556	-.0000014	-.0000103	-.0000964	.0882619

	Orbital	3d	4d
	Energy	-19.16330	-1.36900
ζ_9	8037.8160	.0000113	-.0000042
ζ_{10}	3632.1184	.0000456	-.0000173
ζ_{11}	1715.8784	.0002393	-.0000882
ζ_{12}	839.41314	.0010780	-.0004059
ζ_{13}	421.78083	.0043827	-.0016354
ζ_{14}	216.21547	.0161830	-.0061196
ζ_{15}	112.46515	.0498947	-.0189182
ζ_{16}	59.107083	.1288238	-.0498552
ζ_{17}	31.286316	.2493081	-.0960158
ζ_{18}	16.639226	.3441669	-.1277180
ζ_{19}	8.8764615	.2968723	-.0762922
ζ_{20}	4.7442364	.1220775	.1247470
ζ_{21}	2.5384839	.0208252	.3199560
ζ_{22}	1.3590930	.0010668	.3600344
ζ_{23}	.72788210	.0002432	.2613962
ζ_{24}	.38988551	-.0000846	.1057253
ζ_{25}	.20885248	.0000165	.0298029

Table 51. Sb ^{4}S (28s, 23p, 17d; 28 ζ)

		Symmetry species	S	P	D
		Number of basis functions	28	23	17
Nuclear charge	51	Number of closed shells	5	3	2
No. of electrons	51	Open-shell occupation	0	3	0

Coupling coefficients

$K_0^{pp} = -0.33333333$ $K_2^{pp} = -0.13333333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-6313.485205	-12626.97090	6313.485720	-1.99999991

	Orbital	1s	2s	3s	4s	5s
	Energy	-1085.58897	-164.75791	-33.63617	-6.06314	-0.58175
ζ_1	98892387.	.0000008	-.0000003	.0000001	-.0000001	.0000000
ζ_2	20783995.	.0000042	-.0000014	.0000006	-.0000003	.0000001
ζ_3	4982738.7	.0000239	-.0000077	.0000034	-.0000015	.0000005
ζ_4	1351299.3	.0001109	-.0000359	.0000159	-.0000070	.0000022
ζ_5	410547.29	.0004489	-.0001455	.0000643	-.0000283	.0000088
ζ_6	138227.76	.0015955	-.0005179	.0002289	-.0001007	.0000312
ζ_7	50979.214	.0050567	-.0016473	.0007284	-.0003208	.0000996
ζ_8	20348.676	.0144346	-.0047453	.0021009	-.0009240	.0002868
ζ_9	8686.3120	.0372624	-.0124916	.0055457	-.0024454	.0007599
ζ_{10}	3920.3398	.0861609	-.0301188	.0134508	-.0059232	.0018388
ζ_{11}	1851.0398	.1728270	-.0655811	.0296368	-.0131256	.0040830
ζ_{12}	905.78138	.2799105	-.1244363	.0575674	-.0255074	.0079252
ζ_{13}	455.63794	.3164172	-.1850343	.0894269	-.0402501	.0125665
ζ_{14}	234.02176	.1917618	-.1527932	.0794221	-.0357843	.0111266
ζ_{15}	122.05026	.0399832	.1138352	-.0696137	.0317355	-.0098413
ζ_{16}	64.354540	.0019037	.4997687	-.3980102	.2007738	-.0641255
ζ_{17}	34.192428	-.0001381	.4524056	-.5086046	.2683110	-.0858543
ζ_{18}	18.260492	.0001766	.1175233	.0573454	-.0219490	.0050819
ζ_{19}	9.7846953	-.0002405	.0075699	.7652956	-.6972966	.2531944
ζ_{20}	5.2539923	.0001616	-.0003031	.4544106	-.5897903	.2160764
ζ_{21}	2.8246961	-.0001201	.0004127	.0479221	.4026230	-.1834839
ζ_{22}	1.5196986	.0000928	-.0005898	.0095672	.7609026	-.4220647
ζ_{23}	.81790300	-.0000643	.0003664	-.0032902	.3308662	-.3537638
ζ_{24}	.44027269	.0000439	-.0002685	.0027001	.0159498	.1120338
ζ_{25}	.23701377	-.0000277	.0001740	-.0017178	.0085963	.4740554
ζ_{26}	.12759592	.0000152	-.0000954	.0009255	-.0039413	.5053968
ζ_{27}	.06869152	-.0000064	.0000408	-.0004000	.0019041	.1990312
ζ_{28}	.03698027	.0000015	-.0000095	.0000930	-.0004315	.0180499

Table 51. Sb ^{4}S (28s, 23p, 17d; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-154.00374	-29.10610	-4.44468	-0.33469
ζ_6	138227.76	.0000108	-.0000050	.0000021	-.0000005
ζ_7	50979.214	.0000409	-.0000189	.0000080	-.0000021
ζ_8	20348.676	.0002044	-.0000938	.0000397	-.0000103
ζ_9	8686.3120	.0008169	-.0003781	.0001600	-.0000413
ζ_{10}	3920.3398	.0030164	-.0013937	.0005906	-.0001527
ζ_{11}	1851.0398	.0100538	-.0047039	.0019951	-.0005155
ζ_{12}	905.78138	.0301968	-.0142842	.0060796	-.0015725
ζ_{13}	455.63794	.0804231	-.0392839	.0168044	-.0043479
ζ_{14}	234.02176	.1786423	-.0908540	.0392206	-.0101664
ζ_{15}	122.05026	.3052453	-.1657387	.0724965	-.0188219
ζ_{16}	64.354540	.3396602	-.1859771	.0816083	-.0212101
ζ_{17}	34.192428	.1901987	-.0018109	-.0131724	.0040392
ζ_{18}	18.260492	.0395136	.3561964	-.2146130	.0584921
ζ_{19}	9.7846953	.0023617	.5041061	-.3538752	.0992913
ζ_{20}	5.2539923	.0000218	.2217372	-.0361467	.0004583
ζ_{21}	2.8246961	-.0000341	.0288671	.4303926	-.1476803
ζ_{22}	1.5196986	-.0000996	.0023317	.4966943	-.1869462
ζ_{23}	.81790300	.0000304	.0002311	.2207067	-.0969264
ζ_{24}	.44027269	-.0000318	.0000589	.0293147	.1331806
ζ_{25}	.23701377	.0000199	-.0000257	.0043060	.3490867
ζ_{26}	.12759592	-.0000112	.0000039	-.0007360	.4063556
ζ_{27}	.06869152	.0000052	-.0000027	.0004910	.2341442
ζ_{28}	.03698027	-.0000013	.0000006	-.0001425	.0560664

	Orbital	3d	4d
	Energy	-20.79803	-1.68783
ζ_9	8686.3120	.0000106	-.0000040
ζ_{10}	3920.3398	.0000428	-.0000168
ζ_{11}	1851.0398	.0002248	-.0000862
ζ_{12}	905.78138	.0010139	-.0003959
ζ_{13}	455.63794	.0041185	-.0015961
ζ_{14}	234.02176	.0152404	-.0059803
ζ_{15}	122.05026	.0471938	-.0185793
ζ_{16}	64.354540	.1228352	-.0493373
ζ_{17}	34.192428	.2415413	-.0968206
ζ_{18}	18.260492	.3406133	-.1318632
ζ_{19}	9.7846953	.3038745	-.0856298
ζ_{20}	5.2539923	.1314521	.1165438
ζ_{21}	2.8246961	.0236984	.3230066
ζ_{22}	1.5196986	.0013330	.3699238
ζ_{23}	.81790300	.0002041	.2602896
ζ_{24}	.44027269	-.0000713	.0975578
ζ_{25}	.23701377	.0000069	.0254259

Table 52. Te ^{3}P (28s, 23p, 17d; 28 ζ)

		Symmetry species	S	P	D
		Number of basis functions	28	23	17
Nuclear charge	52	Number of closed shells	5	3	2
No. of electrons	52	Open-shell occupation	0	4	0

Coupling coefficients

$K_0^{pp} = -0.16666667$ $K_2^{pp} = -0.01666667$

Total energy	Potential energy	Kinetic energy	Virial theorem
-6611.783948	-13223.56810	6611.784160	-1.99999997

	Orbital	1s	2s	3s	4s	5s
	Energy	-1130.91694	-172.75537	-35.75485	-6.64698	-0.70054
ζ_1	104930870.	.0000008	-.0000003	.0000001	.0000000	.0000000
ζ_2	22197493.	.0000041	-.0000013	.0000006	-.0000003	.0000001
ζ_3	5344251.0	.0000229	-.0000074	.0000033	-.0000015	.0000005
ζ_4	1452686.7	.0001062	-.0000345	.0000153	-.0000068	.0000022
ζ_5	441685.48	.0004302	-.0001396	.0000619	-.0000276	.0000090
ζ_6	148657.10	.0015310	-.0004976	.0002208	-.0000983	.0000321
ζ_7	54767.020	.0048629	-.0015860	.0007043	-.0003141	.0001027
ζ_8	21830.604	.0139165	-.0045791	.0020356	-.0009066	.0002960
ζ_9	9306.4962	.0360275	-.0120830	.0053869	-.0024055	.0007865
ζ_{10}	4195.9579	.0835925	-.0291991	.0130903	-.0058369	.0019061
ζ_{11}	1980.1464	.1685400	-.0637827	.0289361	-.0129774	.0042478
ζ_{12}	969.04406	.2754832	-.1216277	.0564344	-.0253170	.0082739
ζ_{13}	487.81949	.3172121	-.1832095	.0887799	-.0404603	.0132947
ζ_{14}	250.89218	.1993067	-.1581339	.0821957	-.0374924	.0122581
ζ_{15}	131.10190	.0445870	.0947283	-.0577062	.0264213	-.0085720
ζ_{16}	69.295034	.0021790	.4846616	-.3823680	.1951182	-.0656567
ζ_{17}	36.921593	-.0000531	.4673219	-.5197826	.2772719	-.0933167
ζ_{18}	19.780058	.0001274	.1320738	.0097763	.0075676	-.0052539
ζ_{19}	10.634806	-.0002074	.0088985	.7513293	-.6823491	.2615332
ζ_{20}	5.7307581	.0001358	-.0000969	.4884692	-.6394045	.2480289
ζ_{21}	3.0923192	-.0001020	.0002934	.0571438	.3639529	-.1740115
ζ_{22}	1.6699042	.0000804	-.0005236	.0109073	.7846866	-.4661631
ζ_{23}	.90214456	-.0000556	.0003154	-.0039411	.3478846	-.3912456
ζ_{24}	.48746838	.0000380	-.0002341	.0031854	.0169579	.1481804
ζ_{25}	.26342291	-.0000241	.0001538	-.0020665	.0092337	.5131995
ζ_{26}	.14235542	.0000132	-.0000837	.0011096	-.0040254	.4948354
ζ_{27}	.07693045	-.0000055	.0000359	-.0004810	.0020071	.1716059
ζ_{28}	.04157414	.0000013	-.0000083	.0001113	-.0004446	.0144123

Table 52. Te ^{3}P (28s, 23p, 17d; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-161.73434	-31.08401	-4.95254	-0.35982
ζ_6	148657.10	.0000102	-.0000047	.0000020	-.0000006
ζ_7	54767.020	.0000388	-.0000180	.0000077	-.0000021
ζ_8	21830.604	.0001943	-.0000897	.0000386	-.0000107
ζ_9	9306.4962	.0007787	-.0003621	.0001557	-.0000431
ζ_{10}	4195.9579	.0028820	-.0013388	.0005767	-.0001601
ζ_{11}	1980.1464	.0096228	-.0045236	.0019492	-.0005404
ζ_{12}	969.04406	.0289611	-.0137663	.0059554	-.0016536
ζ_{13}	487.81949	.0773556	-.0379327	.0164850	-.0045774
ζ_{14}	250.89218	.1729557	-.0882947	.0387413	-.0107817
ζ_{15}	131.10190	.2991198	-.1628573	.0723646	-.0201656
ζ_{16}	69.295034	.3412499	-.1890971	.0845707	-.0236171
ζ_{17}	36.921593	.1996561	-.0172355	-.0054565	.0021964
ζ_{18}	19.780058	.0444495	.3386138	-.2078648	.0609495
ζ_{19}	10.634806	.0027734	.5089880	-.3629186	.1098678
ζ_{20}	5.7307581	.0000585	.2381969	-.0609914	.0079767
ζ_{21}	3.0923192	-.0000545	.0329944	.4235762	-.1577955
ζ_{22}	1.6699042	-.0000941	.0028123	.5104583	-.2131784
ζ_{23}	.90214456	.0000246	.0000444	.2254295	-.1007284
ζ_{24}	.48746838	-.0000280	.0001901	.0290751	.1690862
ζ_{25}	.26342291	.0000180	-.0001267	.0046064	.3624918
ζ_{26}	.14235542	-.0000098	.0000538	-.0004852	.3876939
ζ_{27}	.07693045	.0000048	-.0000308	.0006803	.2181956
ζ_{28}	.04157414	-.0000012	.0000064	-.0001018	.0562886

	Orbital	3d	4d
	Energy	-22.51231	-2.03826
ζ_9	9306.4962	.0000100	-.0000040
ζ_{10}	4195.9579	.0000408	-.0000166
ζ_{11}	1980.1464	.0002147	-.0000851
ζ_{12}	969.04406	.0009691	-.0003910
ζ_{13}	487.81949	.0039355	-.0015769
ζ_{14}	250.89218	.0145878	-.0059165
ζ_{15}	131.10190	.0453371	-.0184531
ζ_{16}	69.295034	.1187103	-.0492914
ζ_{17}	36.921593	.2361465	-.0980394
ζ_{18}	19.780058	.3381207	-.1358294
ζ_{19}	10.634806	.3084275	-.0925337
ζ_{20}	5.7307581	.1377888	.1123817
ζ_{21}	3.0923192	.0257189	.3281287
ζ_{22}	1.6699042	.0014956	.3784451
ζ_{23}	.90214456	.0001761	.2561063
ζ_{24}	.48746838	-.0000663	.0887741
ζ_{25}	.26342291	.0000002	.0214171

Table 53. I ^{2}P (28s, 23p, 17d; 28 ζ)

		Symmetry species	S	P	D
		Number of basis functions	28	23	17
Nuclear charge	53	Number of closed shells	5	3	2
No. of electrons	53	Open-shell occupation	0	5	0

Coupling coefficients

$K_0^{pp} = -0.06666667$ $K_2^{pp} = 0.00533333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-6917.980787	-13835.96150	6917.980670	-2.00000002

	Orbital	1s	2s	3s	4s	5s
	Energy	-1177.18625	-180.94919	-37.93444	-7.24433	-0.82110
ζ_1	109066890.	.0000008	-.0000002	.0000001	-.0000001	.0000000
ζ_2	23490798.	.0000039	-.0000013	.0000006	-.0000003	.0000001
ζ_3	5726264.3	.0000219	-.0000071	.0000032	-.0000014	.0000005
ζ_4	1568306.9	.0001008	-.0000327	.0000146	-.0000066	.0000022
ζ_5	478497.32	.0004077	-.0001325	.0000590	-.0000266	.0000091
ζ_6	161092.97	.0014541	-.0004732	.0002108	-.0000950	.0000323
ζ_7	59231.127	.0046409	-.0015153	.0006756	-.0003049	.0001038
ζ_8	23530.844	.0133635	-.0044007	.0019640	-.0008852	.0003009
ζ_9	9991.8892	.0348314	-.0116855	.0052304	-.0023635	.0008046
ζ_{10}	4487.6664	.0813850	-.0284076	.0127831	-.0057686	.0019612
ζ_{11}	2110.9230	.1653075	-.0624175	.0284219	-.0128984	.0043960
ζ_{12}	1030.6417	.2726314	-.1197420	.0557332	-.0253036	.0086090
ζ_{13}	518.19565	.3182611	-.1821842	.0885401	-.0408259	.0139703
ζ_{14}	266.49836	.2048740	-.1619080	.0842776	-.0389217	.0132461
ζ_{15}	139.40229	.0480114	.0817488	-.0497749	.0229382	-.0077081
ζ_{16}	73.832456	.0024307	.4730057	-.3714043	.1916787	-.0672395
ζ_{17}	39.452569	-.0000040	.4767038	-.5266370	.2843286	-.0996461
ζ_{18}	21.211286	.0001015	.1434072	-.0252445	.0294545	-.0137000
ζ_{19}	11.450923	-.0001912	.0101520	.7373789	-.6708741	.2687041
ζ_{20}	6.1981301	.0001232	.0000630	.5142947	-.6782556	.2752144
ζ_{21}	3.3603620	-.0000935	.0001955	.0662932	.3293876	-.1628867
ζ_{22}	1.8235681	.0000750	-.0004700	.0118036	.8048020	-.5066656
ζ_{23}	.99010492	-.0000518	.0002731	-.0042558	.3624696	-.4223557
ζ_{24}	.53771464	.0000354	-.0002049	.0034257	.0186914	.1777648
ζ_{25}	.29205999	-.0000225	.0001371	-.0022607	.0096973	.5381129
ζ_{26}	.15863939	.0000122	-.0000737	.0012050	-.0039626	.4867223
ζ_{27}	.08616991	-.0000051	.0000318	-.0005236	.0020458	.1553365
ζ_{28}	.04680599	.0000012	-.0000073	.0001204	-.0004432	.0125928

Table 53. I ^{2}P (28s, 23p, 17d; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-169.66032	-33.12228	-5.47333	-0.40317
ζ_6	161092.97	.0000095	-.0000044	.0000019	-.0000006
ζ_7	59231.127	.0000364	-.0000170	.0000074	-.0000022
ζ_8	23530.844	.0001834	-.0000851	.0000372	-.0000110
ζ_9	9991.8892	.0007412	-.0003463	.0001511	-.0000445
ζ_{10}	4487.6664	.0027631	-.0012902	.0005643	-.0001663
ζ_{11}	2110.9230	.0092832	-.0043840	.0019176	-.0005645
ζ_{12}	1030.6417	.0280798	-.0134111	.0058902	-.0017370
ζ_{13}	518.19565	.0753052	-.0370785	.0163580	-.0048229
ζ_{14}	266.49836	.1692233	-.0867490	.0386463	-.0114239
ζ_{15}	139.40229	.2948794	-.1611159	.0726826	-.0215097
ζ_{16}	73.832456	.3417486	-.1911022	.0869182	-.0257963
ζ_{17}	39.452569	.2060410	-.0278503	.0000056	.0007314
ζ_{18}	21.211286	.0482930	.3251790	-.2034985	.0635121
ζ_{19}	11.450923	.0031358	.5110164	-.3700511	.1195041
ζ_{20}	6.1981301	.0000938	.2507424	-.0805326	.0147700
ζ_{21}	3.3603620	-.0000774	.0368719	.4173848	-.1668334
ζ_{22}	1.8235681	-.0000850	.0031444	.5217906	-.2377351
ζ_{23}	.99010492	.0000164	-.0000398	.2288652	-.1034429
ζ_{24}	.53771464	-.0000224	.0002467	.0293880	.1962535
ζ_{25}	.29205999	.0000149	-.0001808	.0048870	.3756042
ζ_{26}	.15863939	-.0000077	.0000741	-.0001391	.3771923
ζ_{27}	.08616991	.0000040	-.0000463	.0008188	.2025268
ζ_{28}	.04680599	-.0000009	.0000087	-.0000550	.0512190

	Orbital	3d	4d
	Energy	-24.28566	-2.40118
ζ_9	9991.8892	.0000095	-.0000039
ζ_{10}	4487.6664	.0000391	-.0000164
ζ_{11}	2110.9230	.0002068	-.0000844
ζ_{12}	1030.6417	.0009385	-.0003899
ζ_{13}	518.19565	.0038232	-.0015778
ζ_{14}	266.49836	.0142008	-.0059324
ζ_{15}	139.40229	.0442394	-.0185480
ζ_{16}	73.832456	.1161357	-.0496828
ζ_{17}	39.452569	.2324292	-.0995264
ζ_{18}	21.211286	.3358547	-.1393802
ζ_{19}	11.450923	.3108327	-.0976775
ζ_{20}	6.1981301	.1421970	.1097150
ζ_{21}	3.3603620	.0273756	.3326372
ζ_{22}	1.8235681	.0016151	.3848475
ζ_{23}	.99010492	.0001632	.2512439
ζ_{24}	.53771464	-.0000694	.0817530
ζ_{25}	.29205999	-.0000041	.0189452

Table 54. Xe ^{1}S (28s, 23p, 17d; 28 ζ)

		Symmetry species	S	P	D
		Number of basis functions	28	23	17
Nuclear charge	54	Number of closed shells	5	4	2
No. of electrons	54	Open-shell occupation	0	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-7232.138256	-14464.27750	7232.139210	-1.99999987

	Orbital	1s	2s	3s	4s	5s
	Energy	-1224.39770	-189.34007	-40.17562	-7.85627	-0.94440
ζ_1	115884720.	.0000007	-.0000002	.0000001	.0000000	.0000000
ζ_2	24946026.	.0000038	-.0000012	.0000006	-.0000003	.0000001
ζ_3	6076630.3	.0000214	-.0000069	.0000031	-.0000014	.0000005
ζ_4	1662917.7	.0000982	-.0000320	.0000143	-.0000065	.0000023
ζ_5	506958.58	.0003978	-.0001294	.0000579	-.0000264	.0000093
ζ_6	170557.74	.0014199	-.0004626	.0002069	-.0000943	.0000331
ζ_7	62680.843	.0045342	-.0014823	.0006635	-.0003029	.0001065
ζ_8	24896.214	.0130598	-.0043050	.0019286	-.0008791	.0003089
ζ_9	10573.025	.0340477	-.0114310	.0051365	-.0023475	.0008262
ζ_{10}	4751.0204	.0796052	-.0277847	.0125485	-.0057270	.0020125
ζ_{11}	2236.7438	.1620385	-.0610941	.0279219	-.0128156	.0045158
ζ_{12}	1093.4203	.2687568	-.1174920	.0548509	-.0251842	.0088559
ζ_{13}	550.62399	.3180156	-.1803558	.0878894	-.0409828	.0145021
ζ_{14}	283.70551	.2106291	-.1654764	.0862021	-.0402624	.0141586
ζ_{15}	148.71884	.0522332	.0665836	-.0404597	.0186562	-.0064195
ζ_{16}	78.951008	.0027727	.4586651	-.3576739	.1865260	-.0677299
ζ_{17}	42.293400	.0000743	.4874361	-.5333292	.2909691	-.1053919
ζ_{18}	22.798536	.0000525	.1570103	-.0644088	.0543101	-.0238120
ζ_{19}	12.341394	-.0001557	.0117755	.7210201	-.6557763	.2723566
ζ_{20}	6.6988049	.0000950	.0002521	.5421292	-.7188169	.3027308
ζ_{21}	3.6421288	-.0000733	.0000761	.0761550	.2946243	-.1490791
ζ_{22}	1.9821496	.0000610	-.0003987	.0128658	.8255621	-.5464516
ζ_{23}	1.0793156	-.0000419	.0002169	-.0046662	.3750353	-.4488495
ζ_{24}	.58786286	.0000287	-.0001653	.0037227	.0200405	.2071425
ζ_{25}	.32022498	-.0000183	.0001140	-.0024970	.0101406	.5590915
ζ_{26}	.17444321	.0000099	-.0000603	.0013238	-.0038831	.4786391
ζ_{27}	.09502959	-.0000042	.0000263	-.0005766	.0020706	.1402308
ζ_{28}	.05176841	.0000010	-.0000060	.0001322	-.0004425	.0106234

Table 54. Xe ^{1}S (28s, 23p, 17d; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-177.78239	-35.22162	-6.00831	-0.45728
ζ_6	170557.74	.0000092	-.0000043	.0000019	-.0000006
ζ_7	62680.843	.0000353	-.0000165	.0000073	-.0000022
ζ_8	24896.214	.0001779	-.0000830	.0000368	-.0000113
ζ_9	10573.025	.0007186	-.0003373	.0001493	-.0000458
ζ_{10}	4751.0204	.0026772	-.0012563	.0005578	-.0001714
ζ_{11}	2236.7438	.0089855	-.0042624	.0018920	-.0005806
ζ_{12}	1093.4203	.0271715	-.0130371	.0058122	-.0017874
ζ_{13}	550.62399	.0729280	-.0360460	.0161375	-.0049600
ζ_{14}	283.70551	.1645886	-.0846870	.0382960	-.0118062
ζ_{15}	148.71884	.2894754	-.1586126	.0726083	-.0224035
ζ_{16}	78.951008	.3422345	-.1930894	.0893032	-.0276602
ζ_{17}	42.293400	.2137933	-.0401109	.0065225	-.0012376
ζ_{18}	22.798536	.0529964	.3099230	-.1976372	.0644629
ζ_{19}	12.341394	.0036141	.5135134	-.3773268	.1276607
ζ_{20}	6.6988049	.0001297	.2646583	-.1016238	.0226234
ζ_{21}	3.6421288	-.0000984	.0409828	.4122088	-.1738172
ζ_{22}	1.9821496	-.0000762	.0035379	.5341945	-.2602839
ζ_{23}	1.0793156	.0000091	-.0001808	.2317157	-.1043167
ζ_{24}	.58786286	-.0000175	.0003481	.0289508	.2210057
ζ_{25}	.32022498	.0000113	-.0002399	.0042811	.3898300
ζ_{26}	.17444321	-.0000064	.0001261	-.0006533	.3691344
ζ_{27}	.09502959	.0000030	-.0000585	.0005038	.1861094
ζ_{28}	.05176841	-.0000008	.0000150	-.0001228	.0429509

	Orbital	3d	4d
	Energy	-26.11882	-2.77785
ζ_9	10573.025	.0000092	-.0000038
ζ_{10}	4751.0204	.0000380	-.0000163
ζ_{11}	2236.7438	.0002004	-.0000840
ζ_{12}	1093.4203	.0009076	-.0003871
ζ_{13}	550.62399	.0036900	-.0015636
ζ_{14}	283.70551	.0137038	-.0058782
ζ_{15}	148.71884	.0427878	-.0184215
ζ_{16}	78.951008	.1128396	-.0495730
ζ_{17}	42.293400	.2279718	-.1003818
ζ_{18}	22.798536	.3336194	-.1426328
ζ_{19}	12.341394	.3143023	-.1034708
ζ_{20}	6.6988049	.1474252	.1060696
ζ_{21}	3.6421288	.0291405	.3372964
ζ_{22}	1.9821496	.0017480	.3914827
ζ_{23}	1.0793156	.0001398	.2464803
ζ_{24}	.58786286	-.0000683	.0756934
ζ_{25}	.32022498	-.0000093	.0169010

Table 55-1. Cs ^{2}S (30s, 23p, 17d; 30 ζ)

		Symmetry species	S	P	D
		Number of basis functions	30	23	17
Nuclear charge	55	Number of closed shells	5	4	2
No. of electrons	55	Open-shell occupation	1	0	0

Coupling coefficients

$K_0^{ss} = -1.00000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-7553.933406	-15107.86720	7553.933790	-1.99999995

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1272.76877	-198.14376	-42.69302	-8.69548	-1.23160	-0.12367
ζ_1	87417998.	.0000011	-.0000004	.0000002	-.0000001	.0000000	.0000000
ζ_2	17499618.	.0000066	-.0000021	.0000010	-.0000004	.0000002	.0000000
ζ_3	4062112.1	.0000379	-.0000124	.0000055	-.0000026	.0000009	-.0000002
ζ_4	1081315.5	.0001789	-.0000583	.0000262	-.0000121	.0000045	-.0000010
ζ_5	325908.02	.0007258	-.0002365	.0001062	-.0000489	.0000182	-.0000041
ζ_6	109674.06	.0025642	-.0008376	.0003763	-.0001737	.0000646	-.0000146
ζ_7	40607.212	.0080288	-.0026362	.0011843	-.0005455	.0002026	-.0000459
ζ_8	16300.243	.0225400	-.0075007	.0033789	-.0015612	.0005811	-.0001316
ζ_9	6994.0499	.0567703	-.0194265	.0087780	-.0040459	.0015025	-.0003400
ζ_{10}	3166.2299	.1260450	-.0458019	.0209030	-.0096929	.0036121	-.0008180
ζ_{11}	1494.9207	.2341652	-.0956286	.0443317	-.0205219	.0076231	-.0017252
ζ_{12}	728.90810	.3258637	-.1662365	.0799645	-.0375791	.0140586	-.0031854
ζ_{13}	364.05909	.2715155	-.1945401	.0990575	-.0465499	.0172940	-.0039129
ζ_{14}	185.04984	.0925325	-.0279634	.0159774	-.0088436	.0035989	-.0008269
ζ_{15}	95.241759	.0062435	.3942376	-.2887321	.1506155	-.0578887	.0131659
ζ_{16}	49.445732	.0006894	.5523461	-.5699860	.3104243	-.1185551	.0269100
ζ_{17}	25.820970	-.0003671	.2091670	-.1773610	.1248325	-.0535377	.0123662
ζ_{18}	13.535835	.0001635	.0157419	.7212896	-.6478871	.2849847	-.0659625
ζ_{19}	7.1130915	-.0001498	.0006524	.5910522	-.7890963	.3532043	-.0816029
ζ_{20}	3.7435376	.0001083	-.0002069	.0681365	.3735348	-.1970451	.0457298
ζ_{21}	1.9719170	-.0000712	-.0002154	.0163333	.8701266	-.6727808	.1704607
ζ_{22}	1.0392247	.0000526	.0001072	-.0083729	.2925801	-.3897025	.1009018
ζ_{23}	.54782732	-.0000376	-.0000897	.0064149	.0040617	.4303810	-.1339016
ζ_{24}	.28882433	.0000263	.0000765	-.0047915	.0094237	.6773256	-.2157586
ζ_{25}	.15228219	-.0000184	-.0000519	.0033208	-.0049532	.3242368	-.2439493
ζ_{26}	.08029243	.0000123	.0000362	-.0022649	.0035836	.0102155	-.1336371
ζ_{27}	.04233540	-.0000077	-.0000229	.0014314	-.0022453	.0106772	.2735094
ζ_{28}	.02232203	.0000043	.0000127	-.0007935	.0012425	-.0053891	.6665788
ζ_{29}	.01176966	-.0000018	-.0000054	.0003391	-.0005367	.0027877	.2987659
ζ_{30}	.00620575	.0000004	.0000013	-.0000810	.0001279	-.0006211	.0124963

Table 55-1. Cs ^{2}S (30s, 23p, 17d; 30 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-186.31616	-37.59592	-6.76852	-0.68347
ζ_6	109674.06	.0000213	-.0000100	.0000045	-.0000015
ζ_7	40607.212	.0000792	-.0000371	.0000167	-.0000056
ζ_8	16300.243	.0003935	-.0001852	.0000829	-.0000277
ζ_9	6994.0499	.0015447	-.0007275	.0003279	-.0001099
ζ_{10}	3166.2299	.0056447	-.0026783	.0012022	-.0004018
ζ_{11}	1494.9207	.0184233	-.0088283	.0039896	-.0013380
ζ_{12}	728.90810	.0538873	-.0264424	.0119580	-.0040032
ζ_{13}	364.05909	.1347234	-.0686505	.0314090	-.0105560
ζ_{14}	185.04984	.2660749	-.1437555	.0663572	-.0222990
ζ_{15}	95.241759	.3611744	-.2063648	.0971526	-.0328469
ζ_{16}	49.445732	.2603497	-.0923184	.0343533	-.0108898
ζ_{17}	25.820970	.0718371	.2770505	-.1796936	.0639839
ζ_{18}	13.535835	.0049956	.5431384	-.4022457	.1488380
ζ_{19}	7.1130915	.0000625	.2873155	-.1181261	.0299661
ζ_{20}	3.7435376	-.0000432	.0375754	.4675769	-.2183098
ζ_{21}	1.9719170	-.0001256	.0042340	.5462010	-.3077403
ζ_{22}	1.0392247	.0000526	-.0012313	.1835009	-.0407663
ζ_{23}	.54782732	-.0000454	.0009954	.0147679	.3540541
ζ_{24}	.28882433	.0000316	-.0007068	.0026724	.4750571
ζ_{25}	.15228219	-.0000203	.0004483	-.0007683	.2902537
ζ_{26}	.08029243	.0000117	-.0002582	.0004724	.0572786
ζ_{27}	.04233540	-.0000053	.0001183	-.0002329	.0059176
ζ_{28}	.02232203	.0000014	-.0000314	.0000553	.0005025

	Orbital	3d	4d
	Energy	-28.22621	-3.37953
ζ_9	6994.0499	.0000264	-.0000115
ζ_{10}	3166.2299	.0000970	-.0000417
ζ_{11}	1494.9207	.0005455	-.0002379
ζ_{12}	728.90810	.0023354	-.0010137
ζ_{13}	364.05909	.0096375	-.0042263
ζ_{14}	185.04984	.0332532	-.0146437
ζ_{15}	95.241759	.0970026	-.0434995
ζ_{16}	49.445732	.2166507	-.0980529
ζ_{17}	25.820970	.3429365	-.1514169
ζ_{18}	13.535835	.3389003	-.1190226
ζ_{19}	7.1130915	.1571925	.1148142
ζ_{20}	3.7435376	.0270899	.3760727
ζ_{21}	1.9719170	.0013777	.4087367
ζ_{22}	1.0392247	-.0000396	.2125065
ζ_{23}	.54782732	-.0000032	.0508250
ζ_{24}	.28882433	-.0000248	.0058443
ζ_{25}	.15228219	.0000029	.0004046

Table 55-2. Cs ^{2}S (30s, 22p, 16d; 30 ζ)

		Symmetry species	S	P	D
		Number of basis functions	30	22	16
Nuclear charge	55	Number of closed shells	5	4	2
No. of electrons	55	Open-shell occupation	1	0	0

Coupling coefficients
$K_0^{ss} = -1.00000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-7553.933344	-15107.86730	7553.933920	-1.99999993

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1272.76868	-198.14369	-42.69295	-8.69542	-1.23157	-0.12366
ζ_1	52917903.	.0000021	-.0000007	.0000003	-.0000001	.0000001	.0000000
ζ_2	10685803.	.0000121	-.0000039	.0000018	-.0000008	.0000003	-.0000001
ζ_3	2509778.3	.0000686	-.0000223	.0000100	-.0000046	.0000017	-.0000004
ζ_4	677708.35	.0003167	-.0001031	.0000463	-.0000213	.0000079	-.0000018
ζ_5	207604.88	.0012549	-.0004093	.0001838	-.0000848	.0000315	-.0000071
ζ_6	71100.602	.0043148	-.0014115	.0006338	-.0002923	.0001087	-.0000246
ζ_7	26810.949	.0131010	-.0043226	.0019449	-.0008970	.0003335	-.0000755
ζ_8	10962.849	.0354027	-.0118989	.0053627	-.0024750	.0009202	-.0002083
ζ_9	4790.4172	.0846994	-.0296698	.0134689	-.0062235	.0023148	-.0005240
ζ_{10}	2207.3251	.1740820	-.0661916	.0303603	-.0140668	.0052342	-.0011849
ζ_{11}	1060.0069	.2859413	-.1277688	.0601851	-.0280267	.0104421	-.0023641
ζ_{12}	525.27656	.3224780	-.1907450	.0936994	-.0440800	.0164524	-.0037258
ζ_{13}	266.42596	.1889695	-.1518293	.0812892	-.0389097	.0145892	-.0033056
ζ_{14}	137.42890	.0355700	.1418844	-.0912457	.0451869	-.0170789	.0038736
ζ_{15}	71.736546	.0016247	.5294486	-.4417147	.2341996	-.0895776	.0203476
ζ_{16}	37.753113	-.0003158	.4285097	-.5111719	.2938851	-.1148054	.0261475
ζ_{17}	19.977516	.0002788	.0912844	.1957379	-.1290559	.0517278	-.0118304
ζ_{18}	10.609011	-.0003124	.0048403	.8203473	-.8690209	.3887008	-.0900131
ζ_{19}	5.6465112	.0002247	-.0008498	.3385316	-.4292258	.1891250	-.0437686
ζ_{20}	3.0093649	-.0001633	.0005729	.0305008	.6880460	-.3897123	.0927261
ζ_{21}	1.6051370	.0001254	-.0006980	.0013122	.7279491	-.6844029	.1780918
ζ_{22}	0.8565227	-.0000907	.0004911	.0012834	.1288896	-.1286227	.0263355
ζ_{23}	.45715604	.0000651	-.0003575	-.0011557	.0118245	.5597461	-.1682682
ζ_{24}	.24402706	-.0000465	.0002650	.0007853	-.0036506	.6222803	-.2230072
ζ_{25}	.13026651	.0000323	-.0001841	-.0006256	.0038254	.2001598	-.2303712
ζ_{26}	.06954021	-.0000216	.0001247	.0004268	-.0025358	.0061529	-.0732557
ζ_{27}	.03712291	.0000135	-.0000785	-.0002730	.0016465	.0031629	.3827676
ζ_{28}	.01981750	-.0000074	.0000432	.0001518	-.0009279	-.0010691	.6379739
ζ_{29}	.01057928	.0000031	-.0000183	-.0000643	.0003927	.0007733	.2138000
ζ_{30}	.00564759	-.0000007	.0000043	.0000152	-.0000936	-.0001432	.0049524

Table 55-2. Cs ^{2}S (30s, 22p, 16d; 30 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-186.31609	-37.59586	-6.76846	-0.68343
ζ_5	207604.88	.0000071	-.0000033	.0000015	-.0000005
ζ_6	71100.602	.0000330	-.0000156	.0000070	-.0000024
ζ_7	26810.949	.0001741	-.0000814	.0000364	-.0000121
ζ_8	10962.849	.0007510	-.0003549	.0001601	-.0000537
ζ_9	4790.4172	.0029023	-.0013663	.0006120	-.0002045
ζ_{10}	2207.3251	.0100461	-.0047988	.0021680	-.0007270
ζ_{11}	1060.0069	.0309956	-.0149533	.0067362	-.0022533
ζ_{12}	525.27656	.0841439	-.0420412	.0191622	-.0064356
ζ_{13}	266.42596	.1884345	-.0981148	.0449050	-.0150658
ζ_{14}	137.42890	.3191459	-.1783684	.0834550	-.0281771
ζ_{15}	71.736546	.3394551	-.1863871	.0857489	-.0287337
ζ_{16}	37.753113	.1724085	.0362616	-.0353494	.0129538
ζ_{17}	19.977516	.0294385	.4246786	-.2862173	.1038463
ζ_{18}	10.609011	.0013711	.4881092	-.3675720	.1342678
ζ_{19}	5.6465112	-.0001561	.1587898	.1051829	-.0618593
ζ_{20}	3.0093649	-.0000034	.0171398	.5606161	-.2707094
ζ_{21}	1.6051370	-.0001061	-.0006111	.4373401	-.2620451
ζ_{22}	0.8565227	.0000501	.0013249	.0941935	.0932734
ζ_{23}	.45715604	-.0000354	-.0008903	.0103616	.4072144
ζ_{24}	.24402706	.0000207	.0005126	-.0012125	.4526027
ζ_{25}	.13026651	-.0000093	-.0002416	.0009820	.2062912
ζ_{26}	.06954021	.0000024	.0000650	-.0002971	.0418226

	Orbital	3d	4d
	Energy	-28.22615	-3.37947
ζ_8	10962.849	.0000094	-.0000040
ζ_9	4790.4172	.0000428	-.0000191
ζ_{10}	2207.3251	.0002323	-.0000990
ζ_{11}	1060.0069	.0010897	-.0004789
ζ_{12}	525.27656	.0045635	-.0019770
ζ_{13}	266.42596	.0172139	-.0075934
ζ_{14}	137.42890	.0540856	-.0238971
ζ_{15}	71.736546	.1404879	-.0636305
ζ_{16}	37.753113	.2692354	-.1208323
ζ_{17}	19.977516	.3596329	-.1544681
ζ_{18}	10.609011	.2763603	-.0526116
ζ_{19}	5.6465112	.0921948	.2194891
ζ_{20}	3.0093649	.0117936	.4096128
ζ_{21}	1.6051370	-.0000741	.3569619
ζ_{22}	0.8565227	.0002178	.1415177
ζ_{23}	.45715604	-.0001083	.0344320

Table 56-1. Ba ^{1}S (30s, 23p, 17d; 30 ζ)

		Symmetry species	S	P	D
		Number of basis functions	30	23	17
Nuclear charge	56	Number of closed shells	6	4	2
No. of electrons	56	Open-shell occupation	0	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-7883.543648	-15767.08750	7883.543820	-1.99999998

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1322.09334	-207.15445	-45.28084	-9.55639	-1.51272	-0.15753
ζ_1	69697296.	.0000016	-.0000005	.0000002	-.0000001	.0000000	.0000000
ζ_2	14083979.	.0000089	-.0000029	.0000013	-.0000006	.0000002	-.0000001
ζ_3	3308221.0	.0000508	-.0000166	.0000075	-.0000035	.0000014	-.0000004
ζ_4	893067.69	.0002348	-.0000766	.0000345	-.0000161	.0000063	-.0000017
ζ_5	273471.70	.0009313	-.0003040	.0001369	-.0000638	.0000249	-.0000068
ζ_6	93634.748	.0032077	-.0010498	.0004733	-.0002207	.0000862	-.0000237
ζ_7	35311.107	.0097707	-.0032177	.0014512	-.0006756	.0002635	-.0000726
ζ_8	14446.868	.0266052	-.0088960	.0040242	-.0018786	.0007341	-.0002022
ζ_9	6320.2492	.0647493	-.0223504	.0101469	-.0047280	.0018437	-.0005076
ζ_{10}	2917.5290	.1381257	-.0509285	.0233755	-.0109554	.0042866	-.0011814
ζ_{11}	1404.4903	.2447652	-.1024168	.0478198	-.0223926	.0087351	-.0024049
ζ_{12}	698.09016	.3216687	-.1699071	.0825138	-.0392301	.0154162	-.0042522
ζ_{13}	355.33212	.2512864	-.1858862	.0956914	-.0455298	.0177605	-.0048864
ζ_{14}	184.01595	.0804755	-.0066241	.0037857	-.0029132	.0014525	-.0004242
ζ_{15}	96.468634	.0054016	.3994905	-.2978370	.1574629	-.0636339	.0176407
ζ_{16}	51.001390	.0005116	.5358783	-.5580230	.3082937	-.1238133	.0341909
ζ_{17}	27.116929	-.0002381	.2087480	-.1852142	.1308214	-.0589560	.0166866
ζ_{18}	14.471244	.0000674	.0175523	.6877284	-.6191232	.2870664	-.0813279
ζ_{19}	7.7408083	-.0000804	.0007662	.6122315	-.8187174	.3872918	-.1091436
ζ_{20}	4.1465317	.0000570	-.0002669	.0884933	.2801166	-.1545361	.0429120
ζ_{21}	2.2230268	-.0000337	-.0001743	.0163116	.8839463	-.7026195	.2208512
ζ_{22}	1.1923537	.0000261	.0000589	-.0074793	.3496946	-.4827165	.1542113
ζ_{23}	.63969178	-.0000188	-.0000549	.0059443	.0107759	.4067066	-.1516458
ζ_{24}	.34323202	.0000131	.0000534	-.0045344	.0108960	.7379817	-.3261871
ζ_{25}	.18417376	-.0000092	-.0000351	.0031549	-.0058152	.3296727	-.3399357
ζ_{26}	.09882729	.0000062	.0000249	-.0021641	.0042234	.0090503	.0006156
ζ_{27}	.05303092	-.0000039	-.0000157	.0013677	-.0026524	.0101290	.4173089
ζ_{28}	.02845655	.0000021	.0000087	-.0007543	.0014695	-.0054748	.5930265
ζ_{29}	.01526988	-.0000009	-.0000036	.0003185	-.0006228	.0023679	.2201227
ζ_{30}	.00819387	.0000002	.0000009	-.0000748	.0001467	-.0005662	.0099213

Table 56-1. Ba ^{1}S (30s, 23p, 17d; 30 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-195.05595	-40.03978	-7.54931	-0.90386
ζ_5	273471.70	.0000047	-.0000022	.0000010	-.0000004
ζ_6	93634.748	.0000218	-.0000103	.0000047	-.0000017
ζ_7	35311.107	.0001151	-.0000542	.0000247	-.0000089
ζ_8	14446.868	.0004958	-.0002345	.0001064	-.0000380
ζ_9	6320.2492	.0019249	-.0009113	.0004157	-.0001489
ζ_{10}	2917.5290	.0067069	-.0032009	.0014562	-.0005202
ζ_{11}	1404.4903	.0210628	-.0101624	.0046518	-.0016671
ζ_{12}	698.09016	.0590432	-.0292136	.0133959	-.0047936
ζ_{13}	355.33212	.1413961	-.0727205	.0337283	-.0121173
ζ_{14}	184.01595	.2681520	-.1462809	.0685092	-.0246148
ζ_{15}	96.468634	.3520255	-.2022081	.0964527	-.0348663
ζ_{16}	51.001390	.2507651	-.0863534	.0317663	-.0106526
ζ_{17}	27.116929	.0716944	.2666055	-.1761100	.0672373
ζ_{18}	14.471244	.0054038	.5311186	-.3987088	.1583656
ζ_{19}	7.7408083	.0001660	.2999265	-.1454585	.0440600
ζ_{20}	4.1465317	-.0001127	.0460012	.4320737	-.2187012
ζ_{21}	2.2230268	-.0000798	.0045148	.5603496	-.3386352
ζ_{22}	1.1923537	.0000138	-.0009868	.2111622	-.0765620
ζ_{23}	.63969178	-.0000187	.0008428	.0203918	.3598473
ζ_{24}	.34323202	.0000128	-.0005828	.0028815	.5041416
ζ_{25}	.18417376	-.0000074	.0003311	-.0007522	.2816777
ζ_{26}	.09882729	.0000034	-.0001498	.0003282	.0481561
ζ_{27}	.05303092	-.0000009	.0000405	-.0001384	.0090157

	Orbital	3d	4d
	Energy	-30.40230	-4.00149
ζ_8	14446.868	.0000055	-.0000024
ζ_9	6320.2492	.0000255	-.0000115
ζ_{10}	2917.5290	.0001369	-.0000603
ζ_{11}	1404.4903	.0006518	-.0002909
ζ_{12}	698.09016	.0027395	-.0012168
ζ_{13}	355.33212	.0106939	-.0048009
ζ_{14}	184.01595	.0353222	-.0159266
ζ_{15}	96.468634	.0989999	-.0454832
ζ_{16}	51.001390	.2144963	-.0993724
ζ_{17}	27.116929	.3345457	-.1512569
ζ_{18}	14.471244	.3333482	-.1212798
ζ_{19}	7.7408083	.1619418	.1027079
ζ_{20}	4.1465317	.0309900	.3640408
ζ_{21}	2.2230268	.0017278	.4110451
ζ_{22}	1.1923537	.0000093	.2232807
ζ_{23}	.63969178	-.0000319	.0552665
ζ_{24}	.34323202	-.0000146	.0067611

Table 56-2. Ba ^{1}S (30s, 22p, 16d; 30 ζ)

		Symmetry species	S	P	D
		Number of basis functions	30	22	16
Nuclear charge	56	Number of closed shells	6	4	2
No. of electrons	56	Open-shell occupation	0	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-7883.543542	-15767.08780	7883.544220	-1.99999992

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1322.09325	-207.15437	-45.28077	-9.55632	-1.51268	-0.15751
ζ_1	57649871.	.0000020	-.0000007	.0000003	-.0000001	.0000001	.0000000
ζ_2	11830475.	.0000110	-.0000036	.0000016	-.0000008	.0000003	-.0000001
ζ_3	2805837.2	.0000622	-.0000203	.0000091	-.0000043	.0000017	-.0000005
ζ_4	761000.99	.0002861	-.0000933	.0000420	-.0000196	.0000076	-.0000021
ζ_5	233181.10	.0011372	-.0003713	.0001673	-.0000779	.0000304	-.0000084
ζ_6	79649.999	.0039342	-.0012882	.0005806	-.0002706	.0001056	-.0000291
ζ_7	29905.928	.0120424	-.0039742	.0017941	-.0008359	.0003262	-.0000898
ζ_8	12168.971	.0328455	-.0110309	.0049893	-.0023274	.0009087	-.0002503
ζ_9	5293.3323	.0794153	-.0277277	.0126215	-.0058900	.0022995	-.0006333
ζ_{10}	2430.3389	.1654512	-.0624511	.0287259	-.0134528	.0052573	-.0014483
ζ_{11}	1164.5104	.2774486	-.1220450	.0575263	-.0270377	.0105710	-.0029118
ζ_{12}	576.66042	.3248662	-.1871787	.0919678	-.0437360	.0171513	-.0047279
ζ_{13}	292.73069	.2041514	-.1628177	.0865740	-.0416790	.0163716	-.0045109
ζ_{14}	151.33491	.0440208	.1038063	-.0659467	.0325460	-.0128361	.0035355
ζ_{15}	79.268183	.0020245	.5034543	-.4097405	.2190867	-.0881403	.0243944
ζ_{16}	41.902809	-.0001599	.4599261	-.5358277	.3073635	-.1255373	.0347831
ζ_{17}	22.289769	.0001923	.1161478	.0924365	-.0539547	.0211367	-.0057845
ζ_{18}	11.906123	-.0002586	.0064883	.8085208	-.8305308	.3902972	-.1105330
ζ_{19}	6.3766599	.0001831	-.0004948	.4100094	-.5584660	.2642329	-.0747002
ζ_{20}	3.4208533	-.0001348	.0003878	.0402817	.6039133	-.3537772	.1023959
ζ_{21}	1.8369757	.0001061	-.0006110	.0049975	.7919146	-.7510459	.2423640
ζ_{22}	0.9869957	-.0000769	.0004260	-.0010759	.1743419	-.2210650	.0623540
ζ_{23}	.53046591	.0000554	-.0003146	.0006490	.0112661	.5947950	-.2169168
ζ_{24}	.28514449	-.0000397	.0002386	-.0005639	-.0012215	.6710545	-.3586038
ζ_{25}	.15328601	.0000276	-.0001668	.0003282	.0022478	.1802709	-.2685219
ζ_{26}	.08240478	-.0000185	.0001138	-.0002223	-.0014810	.0050122	.1238341
ζ_{27}	.04430031	.0000116	-.0000719	.0001372	.0009833	.0016887	.5187074
ζ_{28}	.02381564	-.0000063	.0000396	-.0000747	-.0005541	-.0007975	.5203675
ζ_{29}	.01280319	.0000027	-.0000167	.0000313	.0002367	.0003124	.1202012
ζ_{30}	.00688294	-.0000006	.0000039	-.0000073	-.0000559	-.0000707	.0020260

Table 56-2. Ba ^{1}S (30s, 22p, 16d; 30 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-195.05587	-40.03971	-7.54924	-0.90382
ζ_5	233181.10	.0000062	-.0000029	.0000013	-.0000005
ζ_6	79649.999	.0000290	-.0000138	.0000063	-.0000023
ζ_7	29905.928	.0001544	-.0000725	.0000329	-.0000117
ζ_8	12168.971	.0006726	-.0003191	.0001456	-.0000522
ζ_9	5293.3323	.0026234	-.0012405	.0005633	-.0002012
ζ_{10}	2430.3389	.0091540	-.0043877	.0020054	-.0007184
ζ_{11}	1164.5104	.0284590	-.0137737	.0062878	-.0022484
ζ_{12}	576.66042	.0779372	-.0389973	.0179798	-.0064507
ζ_{13}	292.73069	.1771189	-.0922818	.0427837	-.0153452
ζ_{14}	151.33491	.3076968	-.1717630	.0812200	-.0292925
ζ_{15}	79.268183	.3444100	-.1932901	.0908536	-.0326264
ζ_{16}	41.902809	.1910753	.0025108	-.0170754	.0071775
ζ_{17}	22.289769	.0377514	.3877549	-.2626664	.1018457
ζ_{18}	11.906123	.0018992	.5067446	-.3890697	.1533728
ζ_{19}	6.3766599	-.0000871	.1922148	.0380126	-.0371314
ζ_{20}	3.4208533	-.0000355	.0224093	.5416135	-.2810285
ζ_{21}	1.8369757	-.0000998	.0003118	.4751657	-.3059383
ζ_{22}	0.9869957	.0000430	.0008704	.1171171	.0679061
ζ_{23}	.53046591	-.0000317	-.0005801	.0119067	.4373393
ζ_{24}	.28514449	.0000187	.0003275	-.0008296	.4768064
ζ_{25}	.15328601	-.0000085	-.0001555	.0007761	.1790526
ζ_{26}	.08240478	.0000022	.0000434	-.0003022	.0361823

	Orbital	3d	4d
	Energy	-30.40223	-4.00143
ζ_8	12168.971	.0000082	-.0000035
ζ_9	5293.3323	.0000381	-.0000173
ζ_{10}	2430.3389	.0002066	-.0000902
ζ_{11}	1164.5104	.0009795	-.0004398
ζ_{12}	576.66042	.0041071	-.0018203
ζ_{13}	292.73069	.0156144	-.0070405
ζ_{14}	151.33491	.0494337	-.0223298
ζ_{15}	79.268183	.1303143	-.0603170
ζ_{16}	41.902809	.2560514	-.1179293
ζ_{17}	22.289769	.3547706	-.1574521
ζ_{18}	11.906123	.2911602	-.0724439
ζ_{19}	6.3766599	.1073585	.1947623
ζ_{20}	3.4208533	.0153105	.4059337
ζ_{21}	1.8369757	.0001446	.3719682
ζ_{22}	0.9869957	.0001902	.1537155
ζ_{23}	.53046591	-.0001029	.0364142

Table 57-1. La ^{2}F (30s, 23p, 17d, 14f; 30 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	30	23	17	14
Nuclear charge	57	Number of closed shells	6	4	2	0
No. of electrons	57	Open-shell occupation	0	0	0	1

Coupling coefficients

$K_0^{ff} = -1.85714286$ $K_2^{ff} = 0.03809524$ $K_4^{ff} = 0.02597403$ $K_6^{ff} = 0.03330003$

Total energy	Potential energy	Kinetic energy	Virial theorem
-8221.063631	-16442.12730	8221.063650	-2.00000000

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1372.00997	-215.97691	-47.50128	-10.03679	-1.56719	-0.15995
ζ_1	72852697.	.0000016	-.0000005	.0000002	-.0000001	.0000000	.0000000
ζ_2	14886793.	.0000087	-.0000028	.0000013	-.0000006	.0000002	-.0000001
ζ_3	3519889.8	.0000490	-.0000160	.0000072	-.0000034	.0000013	-.0000004
ζ_4	952853.37	.0002261	-.0000738	.0000334	-.0000156	.0000061	-.0000017
ζ_5	291737.18	.0008991	-.0002938	.0001328	-.0000622	.0000242	-.0000066
ζ_6	99675.346	.0031105	-.0010191	.0004611	-.0002161	.0000843	-.0000229
ζ_7	37467.889	.0095254	-.0031400	.0014211	-.0006650	.0002591	-.0000703
ζ_8	15275.462	.0260731	-.0087246	.0039604	-.0018582	.0007254	-.0001969
ζ_9	6661.7045	.0637434	-.0220104	.0100259	-.0046960	.0018295	-.0004964
ζ_{10}	3068.0042	.1364840	-.0503028	.0231662	-.0109122	.0042653	-.0011582
ζ_{11}	1475.1225	.2427282	-.1013854	.0474844	-.0223524	.0087116	-.0023634
ζ_{12}	733.19049	.3208013	-.1687420	.0821961	-.0392750	.0154175	-.0041897
ζ_{13}	373.64229	.2538533	-.1867521	.0963432	-.0460911	.0179663	-.0048717
ζ_{14}	193.94070	.0837238	-.0143662	.0083734	-.0051749	.0023401	-.0006568
ζ_{15}	102.00033	.0059944	.3863598	-.2874841	.1527086	-.0616664	.0168400
ζ_{16}	54.142169	.0005415	.5383416	-.5564514	.3088672	-.1239332	.0337305
ζ_{17}	28.919860	-.0002528	.2212508	-.2150415	.1496508	-.0666860	.0185336
ζ_{18}	15.511799	.0000818	.0201902	.6610091	-.5919522	.2738531	-.0763804
ζ_{19}	8.3423152	-.0000941	.0009279	.6366443	-.8445817	.3997252	-.1110763
ζ_{20}	4.4939518	.0000666	-.0003414	.1025207	.2223916	-.1237446	.0337338
ζ_{21}	2.4232416	-.0000407	-.0001137	.0173195	.8829088	-.6819292	.2093247
ζ_{22}	1.3073949	.0000314	.0000035	-.0075103	.3878525	-.5191437	.1648566
ζ_{23}	.70558012	-.0000225	-.0000163	.0061288	.0157258	.3428656	-.1279021
ζ_{24}	.38084705	.0000156	.0000257	-.0046947	.0124446	.7311758	-.3021326
ζ_{25}	.20558174	-.0000110	-.0000153	.0032771	-.0067617	.3805596	-.3452517
ζ_{26}	.11097641	.0000073	.0000118	-.0022552	.0049734	.0198261	-.0523355
ζ_{27}	.05990749	-.0000045	-.0000074	.0014255	-.0031314	.0110547	.3505382
ζ_{28}	.03233947	.0000025	.0000041	-.0007847	.0017354	-.0059396	.5959943
ζ_{29}	.01745761	-.0000010	-.0000017	.0003300	-.0007334	.0025836	.2914062
ζ_{30}	.00942403	.0000002	.0000004	-.0000770	.0001718	-.0006173	.0228557

Table 57-1. La ^{2}F (30s, 23p, 17d, 14f; 30 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-203.61302	-42.11871	-7.95906	-0.93556
ζ_5	291737.18	.0000045	-.0000021	.0000010	-.0000003
ζ_6	99675.346	.0000209	-.0000099	.0000045	-.0000016
ζ_7	37467.889	.0001110	-.0000526	.0000241	-.0000086
ζ_8	15275.462	.0004817	-.0002287	.0001044	-.0000372
ζ_9	6661.7045	.0018802	-.0008942	.0004106	-.0001468
ζ_{10}	3068.0042	.0065742	-.0031501	.0014418	-.0005138
ζ_{11}	1475.1225	.0206854	-.0100245	.0046184	-.0016517
ζ_{12}	733.19049	.0579979	-.0288053	.0132896	-.0047443
ζ_{13}	373.64229	.1389575	-.0717544	.0334975	-.0120093
ζ_{14}	193.94070	.2641548	-.1445718	.0681241	-.0244184
ζ_{15}	102.00033	.3499982	-.2021352	.0971187	-.0350439
ζ_{16}	54.142169	.2551482	-.0937846	.0360404	-.0121794
ζ_{17}	28.919860	.0763291	.2516904	-.1681541	.0640679
ζ_{18}	15.511799	.0061462	.5279634	-.3982919	.1579808
ζ_{19}	8.3423152	.0002180	.3135610	-.1664886	.0531905
ζ_{20}	4.4939518	-.0001339	.0517601	.4105101	-.2080938
ζ_{21}	2.4232416	-.0000659	.0051012	.5661072	-.3371760
ζ_{22}	1.3073949	.0000008	-.0010328	.2298997	-.0995825
ζ_{23}	.70558012	-.0000106	.0009304	.0243417	.3299793
ζ_{24}	.38084705	.0000076	-.0006396	.0035651	.4987310
ζ_{25}	.20558174	-.0000044	.0003640	-.0009342	.3101151
ζ_{26}	.11097641	.0000020	-.0001647	.0004477	.0610473
ζ_{27}	.05990749	-.0000006	.0000443	-.0001734	.0112721

	Orbital	3d	4d		4f
	Energy	-32.22038	-4.27806		-0.37863
ζ_8	15275.462	.0000054	-.0000024		
ζ_9	6661.7045	.0000250	-.0000113		
ζ_{10}	3068.0042	.0001348	-.0000601		
ζ_{11}	1475.1225	.0006416	-.0002892		
ζ_{12}	733.19049	.0026991	-.0012131		
ζ_{13}	373.64229	.0105039	-.0047664	ζ_{13}	.0001571
ζ_{14}	193.94070	.0346475	-.0158041	ζ_{14}	.0005172
ζ_{15}	102.00033	.0969520	-.0450341	ζ_{15}	.0025005
ζ_{16}	54.142169	.2106495	-.0987962	ζ_{16}	.0094396
ζ_{17}	28.919860	.3307506	-.1515151	ζ_{17}	.0283984
ζ_{18}	15.511799	.3345421	-.1250792	ζ_{18}	.0704557
ζ_{19}	8.3423152	.1672777	.0944003	ζ_{19}	.1454788
ζ_{20}	4.4939518	.0335442	.3572579	ζ_{20}	.2223108
ζ_{21}	2.4232416	.0021098	.4115124	ζ_{21}	.2672202
ζ_{22}	1.3073949	.0000386	.2307869	ζ_{22}	.2620286
ζ_{23}	.70558012	-.0000110	.0595585	ζ_{23}	.2060034
ζ_{24}	.38084705	-.0000124	.0081578	ζ_{24}	.1404260
ζ_{25}	.20558174			ζ_{25}	.0649292
ζ_{26}	.11097641			ζ_{26}	.0308283

Table 57-2. La ^{2}F (29s, 22p, 16d, 13f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	29	22	16	13
Nuclear charge	57	Number of closed shells	6	4	2	0
No. of electrons	57	Open-shell occupation	0	0	0	1

Coupling coefficients

$K_0^{ff} = -1.85714286$ $K_2^{ff} = 0.03809524$ $K_4^{ff} = 0.02597403$ $K_6^{ff} = 0.03330003$

Total energy	Potential energy	Kinetic energy	Virial theorem
-8221.063495	-16442.12740	8221.063860	-1.99999996

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1372.00981	-215.97675	-47.50111	-10.03663	-1.56710	-0.15994
ζ_1	62933525.	.0000019	-.0000006	.0000003	-.0000001	.0000001	.0000000
ζ_2	12646069.	.0000107	-.0000035	.0000016	-.0000007	.0000003	-.0000001
ζ_3	2961111.8	.0000611	-.0000200	.0000090	-.0000042	.0000016	-.0000004
ζ_4	798482.32	.0002823	-.0000922	.0000417	-.0000195	.0000076	-.0000021
ζ_5	244616.35	.0011177	-.0003654	.0001652	-.0000774	.0000302	-.0000082
ζ_6	83874.006	.0038364	-.0012577	.0005688	-.0002665	.0001039	-.0000282
ζ_7	31687.830	.0116311	-.0038420	.0017404	-.0008150	.0003178	-.0000862
ζ_8	12986.344	.0314559	-.0105690	.0047964	-.0022493	.0008773	-.0002381
ζ_9	5687.5891	.0757008	-.0263994	.0120554	-.0056533	.0022048	-.0005983
ζ_{10}	2626.0276	.1581452	-.0594310	.0274105	-.0129047	.0050380	-.0013675
ζ_{11}	1263.0460	.2690188	-.1169931	.0552405	-.0260799	.0101857	-.0027644
ζ_{12}	626.50307	.3255854	-.1837092	.0902707	-.0431461	.0169012	-.0045903
ζ_{13}	317.87962	.2169233	-.1710393	.0907149	-.0438055	.0171882	-.0046665
ζ_{14}	163.92502	.0514429	.0779203	-.0495175	.0242986	-.0095568	.0025921
ζ_{15}	85.494825	.0023479	.4910295	-.3940315	.2114153	-.0849258	.0231554
ζ_{16}	44.933159	.0000029	.4807309	-.5552124	.3191073	-.1301902	.0355424
ζ_{17}	23.734998	.0000791	.1273378	.0629052	-.0337752	.0126702	-.0033847
ζ_{18}	12.577991	-.0001739	.0069282	.8192303	-.8444211	.3959781	-.1104214
ζ_{19}	6.6787344	.0001180	-.0004543	.4192492	-.5690339	.2704730	-.0754300
ζ_{20}	3.5504622	-.0000855	.0003661	.0377946	.6400465	-.3803928	.1089008
ζ_{21}	1.8886914	.0000691	-.0005922	.0057414	.7833759	-.7586370	.2411267
ζ_{22}	1.0050520	-.0000495	.0004140	-.0017713	.1547948	-.1722464	.0447923
ζ_{23}	.53492252	.0000351	-.0003001	.0011129	.0104259	.6351332	-.2277967
ζ_{24}	.28472603	-.0000248	.0002220	-.0008726	-.0017341	.6453659	-.3595329
ζ_{25}	.15155743	.0000166	-.0001490	.0005329	.0023699	.1487044	-.2433219
ζ_{26}	.08067372	-.0000104	.0000946	-.0003366	-.0014679	.0039953	.1603158
ζ_{27}	.04294260	.0000057	-.0000523	.0001843	.0008450	.0005010	.5498986
ζ_{28}	.02285835	-.0000024	.0000222	-.0000780	-.0003657	-.0001241	.4844778
ζ_{29}	.01216750	.0000006	-.0000052	.0000184	.0000876	.0000196	.0920955

Table 57-2. La ^{2}F (29s, 22p, 16d, 13f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-203.61286	-42.11854	-7.95890	-0.93548
ζ_5	244616.35	.0000061	-.0000029	.0000013	-.0000005
ζ_6	83874.006	.0000281	-.0000134	.0000062	-.0000022
ζ_7	31687.830	.0001478	-.0000697	.0000318	-.0000113
ζ_8	12986.344	.0006351	-.0003027	.0001390	-.0000497
ζ_9	5687.5891	.0024518	-.0011637	.0005317	-.0001894
ζ_{10}	2626.0276	.0085065	-.0040943	.0018830	-.0006732
ζ_{11}	1263.0460	.0264595	-.0128445	.0058993	-.0021039
ζ_{12}	626.50307	.0730648	-.0366451	.0169949	-.0060850
ζ_{13}	317.87962	.1690199	-.0881601	.0411137	-.0147076
ζ_{14}	163.92502	.3016365	-.1684954	.0801098	-.0288325
ζ_{15}	85.494825	.3505616	-.1990644	.0944686	-.0338558
ζ_{16}	44.933159	.2027999	-.0128326	-.0088337	.0040931
ζ_{17}	23.734998	.0413338	.3834491	-.2619818	.1015080
ζ_{18}	12.577991	.0020683	.5173384	-.4000466	.1572745
ζ_{19}	6.6787344	-.0001254	.1948878	.0434350	-.0397381
ζ_{20}	3.5504622	-.0000048	.0213441	.5602426	-.2927631
ζ_{21}	1.8886914	-.0001211	.0004051	.4667457	-.2993245
ζ_{22}	1.0050520	.0000605	.0007411	.1049731	.0960932
ζ_{23}	.53492252	-.0000426	-.0005002	.0103032	.4582132
ζ_{24}	.28472603	.0000251	.0002854	-.0010183	.4630787
ζ_{25}	.15155743	-.0000114	-.0001360	.0008036	.1595967
ζ_{26}	.08067372	.0000030	.0000384	-.0003012	.0288910

	Orbital	3d	4d		4f
	Energy	-32.22021	-4.27791		-0.37865
ζ_8	12986.344	.0000077	-.0000033		
ζ_9	5687.5891	.0000354	-.0000164		
ζ_{10}	2626.0276	.0001892	-.0000832		
ζ_{11}	1263.0460	.0008984	-.0004088		
ζ_{12}	626.50307	.0037663	-.0016849		
ζ_{13}	317.87962	.0145189	-.0066238	ζ_{13}	.0002391
ζ_{14}	163.92502	.0467862	-.0213483	ζ_{14}	.0007746
ζ_{15}	85.494825	.1262683	-.0591033	ζ_{15}	.0037727
ζ_{16}	44.933159	.2543462	-.1185979	ζ_{16}	.0137006
ζ_{17}	23.734998	.3592982	-.1617778	ζ_{17}	.0392275
ζ_{18}	12.577991	.2965769	-.0742972	ζ_{18}	.0945406
ζ_{19}	6.6787344	.1071410	.2045990	ζ_{19}	.1795101
ζ_{20}	3.5504622	.0144171	.4187979	ζ_{20}	.2488801
ζ_{21}	1.8886914	.0001316	.3667171	ζ_{21}	.2800019
ζ_{22}	1.0050520	.0001961	.1423080	ζ_{22}	.2443799
ζ_{23}	.53492252	-.0000827	.0302674	ζ_{23}	.1873290
ζ_{24}	.28472603			ζ_{24}	.0952277
ζ_{25}	.15155743			ζ_{25}	.0600762

Table 58-1. Ce ^{3}H (30s, 23p, 17d, 14f; 30 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	30	23	17	14
Nuclear charge	58	Number of closed shells	6	4	2	0
No. of electrons	58	Open-shell occupation	0	0	0	2

Coupling coefficients

$K_0^{ff} = -0.85714286$ $K_2^{ff} = -0.07301587$ $K_4^{ff} = -0.02085793$ $K_6^{ff} = 0.03153412$

Total energy	Potential energy	Kinetic energy	Virial theorem
-8566.919396	-17133.83930	8566.919900	-1.99999994

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1422.82819	-224.94794	-49.72899	-10.49545	-1.61356	-0.16201
ζ_1	76389852.	.0000015	-.0000005	.0000002	-.0000001	.0000000	.0000000
ζ_2	15595632.	.0000085	-.0000028	.0000013	-.0000006	.0000002	-.0000001
ζ_3	3685365.7	.0000484	-.0000158	.0000072	-.0000034	.0000013	-.0000004
ζ_4	997350.55	.0002232	-.0000729	.0000331	-.0000156	.0000061	-.0000016
ζ_5	305339.90	.0008872	-.0002903	.0001316	-.0000619	.0000240	-.0000064
ζ_6	104334.15	.0030687	-.0010066	.0004570	-.0002151	.0000836	-.0000224
ζ_7	39228.213	.0093948	-.0031004	.0014077	-.0006615	.0002569	-.0000688
ζ_8	15998.011	.0257134	-.0086125	.0039223	-.0018480	.0007188	-.0001926
ζ_9	6979.1449	.0628891	-.0217284	.0099297	-.0046700	.0018130	-.0004856
ζ_{10}	3215.2600	.1348438	-.0496947	.0229589	-.0108592	.0042296	-.0011337
ζ_{11}	1546.3910	.2405887	-.1003428	.0471399	-.0222813	.0086536	-.0023176
ζ_{12}	768.81306	.3201036	-.1677477	.0819361	-.0393118	.0153771	-.0041248
ζ_{13}	391.87875	.2565145	-.1878282	.0971481	-.0466736	.0181330	-.0048542
ζ_{14}	203.43960	.0864809	-.0200850	.0116969	-.0068431	.0029840	-.0008198
ζ_{15}	107.00887	.0063958	.3797524	-.2826477	.1507884	-.0606795	.0163545
ζ_{16}	56.805331	.0005759	.5414343	-.5593894	.3120054	-.1248156	.0335387
ζ_{17}	30.343907	-.0002778	.2270907	-.2265632	.1576502	-.0697437	.0191058
ζ_{18}	16.276049	.0001031	.0209595	.6592663	-.5947205	.2742084	-.0754483
ζ_{19}	8.7534092	-.0001109	.0010199	.6423465	-.8532749	.4027981	-.1105029
ζ_{20}	4.7153878	.0000793	-.0004157	.1040287	.2255123	-.1260137	.0340607
ζ_{21}	2.5426140	-.0000502	-.0000530	.0174359	.8837244	-.6804021	.2055307
ζ_{22}	1.3717750	.0000383	-.0000406	-.0075659	.3870062	-.5129953	.1607585
ζ_{23}	.74030957	-.0000275	.0000164	.0061803	.0161194	.3360410	-.1232301
ζ_{24}	.39958371	.0000192	.0000020	-.0047272	.0122949	.7244274	-.2925306
ζ_{25}	.21569072	-.0000135	.0000014	.0033024	-.0066556	.3867647	-.3404394
ζ_{26}	.11643060	.0000090	.0000005	-.0022726	.0049086	.0223744	-.0632263
ζ_{27}	.06285026	-.0000056	-.0000004	.0014366	-.0030903	.0109847	.3327582
ζ_{28}	.03392722	.0000030	.0000002	-.0007909	.0017131	-.0058918	.5914506
ζ_{29}	.01831427	-.0000013	-.0000001	.0003326	-.0007240	.0025686	.3097918
ζ_{30}	.00988624	.0000003	.0000000	-.0000776	.0001696	-.0006145	.0276530

Table 58-1. Ce ^{3}H (30s, 23p, 17d, 14f; 30 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-212.31908	-44.20475	-8.34781	-0.96109
ζ_5	305339.90	.0000044	-.0000021	.0000010	-.0000003
ζ_6	104334.15	.0000205	-.0000098	.0000045	-.0000016
ζ_7	39228.213	.0001091	-.0000519	.0000239	-.0000085
ζ_8	15998.011	.0004731	-.0002256	.0001035	-.0000366
ζ_9	6979.1449	.0018464	-.0008817	.0004069	-.0001447
ζ_{10}	3215.2600	.0064556	-.0031059	.0014287	-.0005064
ζ_{11}	1546.3910	.0203275	-.0098902	.0045794	-.0016289
ζ_{12}	768.81306	.0570781	-.0284579	.0131954	-.0046855
ζ_{13}	391.87875	.1371832	-.0711008	.0333614	-.0118960
ζ_{14}	203.43960	.2620720	-.1439677	.0681913	-.0243135
ζ_{15}	107.00887	.3499648	-.2030586	.0980980	-.0352075
ζ_{16}	56.805331	.2580624	-.0976981	.0383134	-.0129448
ζ_{17}	30.343907	.0782687	.2488511	-.1679750	.0637402
ζ_{18}	16.276049	.0063376	.5298130	-.4025951	.1588733
ζ_{19}	8.7534092	.0002300	.3153563	-.1672081	.0530775
ζ_{20}	4.7153878	-.0001439	.0519447	.4146323	-.2096295
ζ_{21}	2.5426140	-.0000571	.0051267	.5653955	-.3346589
ζ_{22}	1.3717750	-.0000042	-.0010338	.2279723	-.0962495
ζ_{23}	.74030957	-.0000068	.0009416	.0241104	.3264419
ζ_{24}	.39958371	.0000052	-.0006429	.0035211	.4945343
ζ_{25}	.21569072	-.0000031	.0003666	-.0009007	.3133828
ζ_{26}	.11643060	.0000014	-.0001659	.0004402	.0635885
ζ_{27}	.06285026	-.0000004	.0000445	-.0001695	.0116438

	Orbital	3d	4d		4f
	Energy	-34.04564	-4.53587		-0.47337
ζ_8	15998.011	.0000053	-.0000024		
ζ_9	6979.1449	.0000246	-.0000112		
ζ_{10}	3215.2600	.0001329	-.0000597		
ζ_{11}	1546.3910	.0006328	-.0002880		
ζ_{12}	768.81306	.0026629	-.0012074		
ζ_{13}	391.87875	.0103799	-.0047537	ζ_{13}	.0001660
ζ_{14}	203.43960	.0343375	-.0158054	ζ_{14}	.0005473
ζ_{15}	107.00887	.0964413	-.0452193	ζ_{15}	.0026549
ζ_{16}	56.805331	.2104292	-.0996503	ζ_{16}	.0100435
ζ_{17}	30.343907	.3316362	-.1534904	ζ_{17}	.0303311
ζ_{18}	16.276049	.3351863	-.1258041	ζ_{18}	.0753407
ζ_{19}	8.7534092	.1664830	.0982869	ζ_{19}	.1544500
ζ_{20}	4.7153878	.0329911	.3618699	ζ_{20}	.2328241
ζ_{21}	2.5426140	.0021034	.4101635	ζ_{21}	.2748835
ζ_{22}	1.3717750	.0000732	.2264678	ζ_{22}	.2606575
ζ_{23}	.74030957	.0000008	.0575303	ζ_{23}	.1969769
ζ_{24}	.39958371	-.0000073	.0079468	ζ_{24}	.1242983
ζ_{25}	.21569072			ζ_{25}	.0535222
ζ_{26}	.11643060			ζ_{26}	.0197300

Table 58-2. Ce ^{3}H (29s, 22p, 16d, 13f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	29	22	16	13
Nuclear charge	58	Number of closed shells	6	4	2	0
No. of electrons	58	Open-shell occupation	0	0	0	2

Coupling coefficients

$K_0^{ff} = -0.85714286$ $K_2^{ff} = -0.07301587$ $K_4^{ff} = -0.02085793$ $K_6^{ff} = 0.03153412$

Total energy	Potential energy	Kinetic energy	Virial theorem
-8566.919256	-17133.83830	8566.919030	-2.00000003

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1422.82809	-224.94784	-49.72888	-10.49533	-1.61349	-0.16200
ζ_1	66258147.	.0000018	-.0000006	.0000003	-.0000001	.0000000	.0000000
ζ_2	13273362.	.0000106	-.0000035	.0000016	-.0000007	.0000003	-.0000001
ζ_3	3102048.6	.0000603	-.0000197	.0000089	-.0000042	.0000016	-.0000004
ζ_4	835711.21	.0002787	-.0000911	.0000413	-.0000194	.0000076	-.0000020
ζ_5	255987.02	.0011029	-.0003609	.0001638	-.0000770	.0000299	-.0000080
ζ_6	87812.103	.0037821	-.0012413	.0005633	-.0002650	.0001030	-.0000276
ζ_7	33202.903	.0114526	-.0037871	.0017212	-.0008093	.0003144	-.0000842
ζ_8	13620.921	.0309447	-.0104065	.0047382	-.0022312	.0008672	-.0002323
ζ_9	5971.6632	.0744620	-.0259762	.0119004	-.0056033	.0021776	-.0005833
ζ_{10}	2759.7866	.1558047	-.0585142	.0270714	-.0127982	.0049790	-.0013341
ζ_{11}	1328.4179	.2662517	-.1154635	.0546743	-.0259160	.0100858	-.0027021
ζ_{12}	659.31537	.3255165	-.1825861	.0899371	-.0431656	.0168500	-.0045176
ζ_{13}	334.65685	.2210622	-.1735919	.0922316	-.0447093	.0174801	-.0046846
ζ_{14}	172.61081	.0542428	.0687042	-.0438976	.0215448	-.0084339	.0022569
ζ_{15}	90.028063	.0025154	.4845963	-.3880262	.2090431	-.0836859	.0225236
ζ_{16}	47.311089	.0000590	.4881274	-.5629860	.3249608	-.1321200	.0356012
ζ_{17}	24.986106	.0000406	.1330393	.0473910	-.0236225	.0083502	-.0021678
ζ_{18}	13.237353	-.0001454	.0071920	.8211930	-.8495645	.3969483	-.1092288
ζ_{19}	7.0265379	.0000967	-.0003655	.4270743	-.5789109	.2744937	-.0755279
ζ_{20}	3.7339966	-.0000698	.0003097	.0385547	.6416103	-.3811450	.1076308
ζ_{21}	1.9855552	.0000578	-.0005520	.0060182	.7840614	-.7536645	.2357077
ζ_{22}	1.0561741	-.0000414	.0003865	-.0019570	.1564116	-.1731420	.0450950
ζ_{23}	.56190214	.0000294	-.0002810	.0012588	.0101281	.6244414	-.2199317
ζ_{24}	.29896346	-.0000208	.0002088	-.0009725	-.0014289	.6463984	-.3500875
ζ_{25}	.15907009	.0000139	-.0001402	.0006014	.0021623	.1554025	-.2467294
ζ_{26}	.08463762	-.0000088	.0000891	-.0003801	-.0013302	.0039639	.1440136
ζ_{27}	.04503391	.0000048	-.0000493	.0002084	.0007677	.0008008	.5357725
ζ_{28}	.02396162	-.0000020	.0000209	-.0000882	-.0003326	-.0002547	.4962579
ζ_{29}	.01274949	.0000005	-.0000050	.0000209	.0000797	.0000511	.1045229

Table 58-2. Ce ^{3}H (29s, 22p, 16d, 13f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-212.31898	-44.20463	-8.34769	-0.96102
ζ_5	255987.02	.0000060	-.0000028	.0000013	-.0000005
ζ_6	87812.103	.0000276	-.0000132	.0000061	-.0000022
ζ_7	33202.903	.0001449	-.0000686	.0000314	-.0000111
ζ_8	13620.921	.0006217	-.0002976	.0001373	-.0000488
ζ_9	5971.6632	.0023969	-.0011423	.0005246	-.0001858
ζ_{10}	2759.7866	.0083098	-.0040158	.0018561	-.0006601
ζ_{11}	1328.4179	.0258616	-.0126027	.0058174	-.0020636
ζ_{12}	659.31537	.0715578	-.0360198	.0167880	-.0059786
ζ_{13}	334.65685	.1663036	-.0870401	.0407979	-.0145168
ζ_{14}	172.61081	.2990325	-.1675953	.0800829	-.0286678
ζ_{15}	90.028063	.3518432	-.2011442	.0960636	-.0342561
ζ_{16}	47.311089	.2071084	-.0190184	-.0055684	.0028915
ζ_{17}	24.986106	.0430711	.3803220	-.2620565	.1010559
ζ_{18}	13.237353	.0021518	.5208781	-.4051962	.1585435
ζ_{19}	7.0265379	-.0001223	.1974574	.0426710	-.0395204
ζ_{20}	3.7339966	-.0000041	.0215641	.5627258	-.2929179
ζ_{21}	1.9855552	-.0001213	.0004686	.4658541	-.2959843
ζ_{22}	1.0561741	.0000616	.0007200	.1046733	.0956793
ζ_{23}	.56190214	-.0000432	-.0004789	.0101715	.4526017
ζ_{24}	.29896346	.0000255	.0002749	-.0009429	.4630664
ζ_{25}	.15907009	-.0000116	-.0001311	.0007792	.1638911
ζ_{26}	.08463762	.0000030	.0000370	-.0002904	.0300745

	Orbital	3d	4d		4f
	Energy	-34.04552	-4.53576		-0.47333
ζ_8	13620.921	.0000076	-.0000033		
ζ_9	5971.6632	.0000347	-.0000162		
ζ_{10}	2759.7866	.0001853	-.0000821		
ζ_{11}	1328.4179	.0008796	-.0004040		
ζ_{12}	659.31537	.0036876	-.0016643		
ζ_{13}	334.65685	.0142515	-.0065613	ζ_{13}	.0002496
ζ_{14}	172.61081	.0461140	-.0212337	ζ_{14}	.0008158
ζ_{15}	90.028063	.1251344	-.0591188	ζ_{15}	.0039683
ζ_{16}	47.311089	.2537315	-.1195062	ζ_{16}	.0145160
ζ_{17}	24.986106	.3603097	-.1638904	ζ_{17}	.0417094
ζ_{18}	13.237353	.2976136	-.0745999	ζ_{18}	.1006977
ζ_{19}	7.0265379	.1069560	.2085778	ζ_{19}	.1892659
ζ_{20}	3.7339966	.0142773	.4215454	ζ_{20}	.2594282
ζ_{21}	1.9855552	.0001825	.3639970	ζ_{21}	.2841808
ζ_{22}	1.0561741	.0002147	.1391920	ζ_{22}	.2407708
ζ_{23}	.56190214	-.0000705	.0293844	ζ_{23}	.1722112
ζ_{24}	.29896346			ζ_{24}	.0843263
ζ_{25}	.15907009			ζ_{25}	.0425337

Table 59-1. Pr ^{4}I (30s, 23p, 17d, 14f; 30 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	30	23	17	14
Nuclear charge	59	Number of closed shells	6	4	2	0
No. of electrons	59	Open-shell occupation	0	0	0	3

Coupling coefficients

$K_0^{ff} = -0.52380952$ $K_2^{ff} = -0.09029982$ $K_4^{ff} = -0.03157112$ $K_6^{ff} = 0.01995760$

Total energy	Potential energy	Kinetic energy	Virial theorem
-8921.180837	-17842.36250	8921.181660	-1.99999991

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1474.55934	-234.08023	-51.97888	-10.94517	-1.65628	-0.16392
ζ_1	80038348.	.0000015	-.0000005	.0000002	-.0000001	.0000000	.0000000
ζ_2	16370891.	.0000084	-.0000027	.0000012	-.0000006	.0000002	-.0000001
ζ_3	3872650.6	.0000474	-.0000155	.0000071	-.0000033	.0000013	-.0000003
ζ_4	1048452.2	.0002188	-.0000716	.0000326	-.0000154	.0000060	-.0000016
ζ_5	320954.26	.0008704	-.0002851	.0001297	-.0000612	.0000236	-.0000063
ζ_6	109623.82	.0030130	-.0009895	.0004506	-.0002128	.0000823	-.0000218
ζ_7	41193.403	.0092340	-.0030505	.0013894	-.0006551	.0002532	-.0000670
ζ_8	16789.634	.0253029	-.0084824	.0038751	-.0018319	.0007093	-.0001879
ζ_9	7320.9909	.0619713	-.0214214	.0098194	-.0046340	.0017908	-.0004742
ζ_{10}	3371.7731	.1331405	-.0490552	.0227317	-.0107884	.0041827	-.0011082
ζ_{11}	1621.5827	.2383656	-.0992471	.0467571	-.0221761	.0085737	-.0022700
ζ_{12}	806.35910	.3192592	-.1666226	.0815956	-.0392805	.0152937	-.0040551
ζ_{13}	411.20179	.2592049	-.1887890	.0978551	-.0471800	.0182496	-.0048303
ζ_{14}	213.61519	.0895535	-.0264545	.0154357	-.0087207	.0037003	-.0009988
ζ_{15}	112.45891	.0069109	.3709897	-.2759306	.1476976	-.0591637	.0157600
ζ_{16}	59.759874	.0006096	.5441197	-.5605363	.3137659	-.1249807	.0332036
ζ_{17}	31.958974	-.0002997	.2350608	-.2432456	.1685746	-.0738637	.0199677
ζ_{18}	17.163744	.0001230	.0224139	.6494372	-.5871644	.2692779	-.0731861
ζ_{19}	9.2429735	-.0001275	.0011309	.6532610	-.8652854	.4068154	-.1103406
ζ_{20}	4.9859050	.0000918	-.0004851	.1094747	.2092346	-.1175939	.0314803
ζ_{21}	2.6922343	-.0000595	.0000063	.0178546	.8819224	-.6689531	.1987216
ζ_{22}	1.4545539	.0000453	-.0000876	-.0076013	.3989410	-.5196839	.1612802
ζ_{23}	.78610396	-.0000326	.0000505	.0062660	.0182275	.3092260	-.1124495
ζ_{24}	.42491000	.0000229	-.0000230	-.0047921	.0127057	.7154868	-.2796220
ζ_{25}	.22969136	-.0000161	.0000190	.0033523	-.0069060	.4074495	-.3376486
ζ_{26}	.12416667	.0000107	-.0000114	-.0023091	.0051207	.0291448	-.0847456
ζ_{27}	.06712278	-.0000067	.0000071	.0014597	-.0032262	.0110871	.3021106
ζ_{28}	.03628576	.0000036	-.0000039	-.0008033	.0017892	-.0058892	.5832396
ζ_{29}	.01961565	-.0000015	.0000016	.0003375	-.0007558	.0025780	.3425300
ζ_{30}	.01060399	.0000003	-.0000004	-.0000787	.0001769	-.0006175	.0378859

Table 59-1. Pr ^{4}I (30s, 23p, 17d, 14f; 30 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-221.18657	-46.31268	-8.72783	-0.98382
ζ_5	320954.26	.0000043	-.0000020	.0000009	-.0000003
ζ_6	109623.82	.0000200	-.0000096	.0000044	-.0000015
ζ_7	41193.403	.0001067	-.0000509	.0000236	-.0000083
ζ_8	16789.634	.0004630	-.0002216	.0001021	-.0000359
ζ_9	7320.9909	.0018089	-.0008673	.0004020	-.0001420
ζ_{10}	3371.7731	.0063294	-.0030568	.0014119	-.0004971
ζ_{11}	1621.5827	.0199511	-.0097444	.0045312	-.0016011
ζ_{12}	806.35910	.0560889	-.0280637	.0130663	-.0046088
ζ_{13}	411.20179	.1351559	-.0702945	.0331252	-.0117338
ζ_{14}	213.61519	.2593657	-.1429440	.0679910	-.0240816
ζ_{15}	112.45891	.3493222	-.2036011	.0988294	-.0352392
ζ_{16}	59.759874	.2614647	-.1026271	.0411630	-.0138910
ζ_{17}	31.958974	.0811048	.2423194	-.1650938	.0622768
ζ_{18}	17.163744	.0067290	.5299712	-.4047182	.1586678
ζ_{19}	9.2429735	.0002543	.3207036	-.1738779	.0555675
ζ_{20}	4.9859050	-.0001557	.0538797	.4099659	-.2063102
ζ_{21}	2.6922343	-.0000472	.0053467	.5661356	-.3309539
ζ_{22}	1.4545539	-.0000114	-.0010504	.2331017	-.1019025
ζ_{23}	.78610396	-.0000019	.0009791	.0253680	.3133599
ζ_{24}	.42491000	.0000021	-.0006644	.0037350	.4890658
ζ_{25}	.22969136	-.0000013	.0003793	-.0009511	.3249304
ζ_{26}	.12416667	.0000006	-.0001717	.0004794	.0705294
ζ_{27}	.06712278	-.0000002	.0000460	-.0001798	.0128861

	Orbital	3d	4d		4f
	Energy	-35.89246	-4.78574		-0.54920
ζ_8	16789.634	.0000052	-.0000024		
ζ_9	7320.9909	.0000242	-.0000111		
ζ_{10}	3371.7731	.0001307	-.0000592		
ζ_{11}	1621.5827	.0006225	-.0002854		
ζ_{12}	806.35910	.0026214	-.0011978		
ζ_{13}	411.20179	.0102223	-.0047173	ζ_{13}	.0001721
ζ_{14}	213.61519	.0338836	-.0157191	ζ_{14}	.0005671
ζ_{15}	112.45891	.0954073	-.0450842	ζ_{15}	.0027559
ζ_{16}	59.759874	.2090621	-.0998398	ζ_{16}	.0104310
ζ_{17}	31.958974	.3311002	-.1546372	ζ_{17}	.0316032
ζ_{18}	17.163744	.3360754	-.1273403	ζ_{18}	.0785277
ζ_{19}	9.2429735	.1676659	.0980068	ζ_{19}	.1600778
ζ_{20}	4.9859050	.0334414	.3621365	ζ_{20}	.2390473
ζ_{21}	2.6922343	.0022322	.4093010	ζ_{21}	.2784196
ζ_{22}	1.4545539	.0001042	.2267132	ζ_{22}	.2584787
ζ_{23}	.78610396	.0000160	.0579690	ζ_{23}	.1903064
ζ_{24}	.42491000	-.0000045	.0082751	ζ_{24}	.1151072
ζ_{25}	.22969136			ζ_{25}	.0473223
ζ_{26}	.12416667			ζ_{26}	.0153318

Table 59-2. Pr ^{4}I (29s, 22p, 16d, 13f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	29	22	16	13
Nuclear charge	59	Number of closed shells	6	4	2	0
No. of electrons	59	Open-shell occupation	0	0	0	3

Coupling coefficients

$K_0^{ff} = -0.52380952$ $K_2^{ff} = -0.09029982$ $K_4^{ff} = -0.03157112$ $K_6^{ff} = 0.01995760$

Total energy	Potential energy	Kinetic energy	Virial theorem
-8921.180691	-17842.36190	8921.181180	-1.99999995

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1474.55923	-234.08013	-51.97877	-10.94505	-1.65622	-0.16390
ζ_1	68140110.	.0000019	-.0000006	.0000003	-.0000001	.0000001	.0000000
ζ_2	13763471.	.0000105	-.0000034	.0000016	-.0000007	.0000003	-.0000001
ζ_3	3232397.4	.0000597	-.0000195	.0000089	-.0000042	.0000016	-.0000004
ζ_4	872661.74	.0002754	-.0000901	.0000410	-.0000194	.0000075	-.0000020
ζ_5	267288.60	.0010917	-.0003577	.0001628	-.0000768	.0000297	-.0000079
ζ_6	91546.203	.0037555	-.0012340	.0005617	-.0002651	.0001026	-.0000272
ζ_7	34531.867	.0114158	-.0037792	.0017230	-.0008130	.0003144	-.0000833
ζ_8	14128.469	.0309563	-.0104222	.0047601	-.0022490	.0008702	-.0002305
ζ_9	6178.9780	.0746904	-.0260887	.0119904	-.0056658	.0021920	-.0005804
ζ_{10}	2850.0951	.1564622	-.0588541	.0273171	-.0129577	.0050179	-.0013292
ζ_{11}	1370.2289	.2671515	-.1161275	.0551839	-.0262554	.0101723	-.0026940
ζ_{12}	679.78154	.3255584	-.1832162	.0905846	-.0436266	.0169516	-.0044929
ζ_{13}	345.16717	.2199290	-.1731565	.0924306	-.0450092	.0175232	-.0046423
ζ_{14}	178.21923	.0536098	.0707844	-.0455353	.0225309	-.0087937	.0023264
ζ_{15}	93.106192	.0024963	.4850850	-.3908430	.2114800	-.0842841	.0224250
ζ_{16}	49.032593	.0000372	.4866295	-.5646489	.3281521	-.1329411	.0354111
ζ_{17}	25.959773	.0000559	.1327831	.0503808	-.0269110	.0098572	-.0025478
ζ_{18}	13.791156	-.0001567	.0071268	.8222894	-.8579044	.3992525	-.1085799
ζ_{19}	7.3420953	.0001060	-.0003342	.4257617	-.5746204	.2709957	-.0736376
ζ_{20}	3.9136900	-.0000770	.0002864	.0395645	.6399610	-.3789972	.1056497
ζ_{21}	2.0876759	.0000632	-.0005324	.0055873	.7824365	-.7437126	.2292068
ζ_{22}	1.1140532	-.0000454	.0003732	-.0016024	.1607176	-.1821988	.0481572
ζ_{23}	.59460959	.0000323	-.0002722	.0010154	.0102685	.6005831	-.2077179
ζ_{24}	.31739203	-.0000229	.0002027	-.0007958	-.0011869	.6527951	-.3385707
ζ_{25}	.16942433	.0000154	-.0001361	.0004794	.0020318	.1718523	-.2549412
ζ_{26}	.09044012	-.0000097	.0000865	-.0003026	-.0012361	.0046984	.1123617
ζ_{27}	.04827787	.0000053	-.0000477	.0001649	.0007154	.0012611	.5094370
ζ_{28}	.02577125	-.0000022	.0000202	-.0000695	-.0003096	-.0004552	.5156213
ζ_{29}	.01375697	.0000005	-.0000048	.0000164	.0000740	.0000993	.1335151

Table 59-2. Pr ^{4}I (29s, 22p, 16d, 13f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-221.18647	-46.31256	-8.72772	-0.98375
ζ_5	267288.60	.0000059	-.0000028	.0000013	-.0000005
ζ_6	91546.203	.0000274	-.0000131	.0000061	-.0000022
ζ_7	34531.867	.0001444	-.0000686	.0000316	-.0000111
ζ_8	14128.469	.0006225	-.0002991	.0001386	-.0000490
ζ_9	6178.9780	.0024095	-.0011529	.0005316	-.0001871
ζ_{10}	2850.0951	.0083752	-.0040636	.0018863	-.0006663
ζ_{11}	1370.2289	.0260912	-.0127685	.0059187	-.0020858
ζ_{12}	679.78154	.0721294	-.0364680	.0170733	-.0060398
ζ_{13}	345.16717	.1672189	-.0879390	.0414021	-.0146360
ζ_{14}	178.21923	.2995517	-.1687532	.0810343	-.0288186
ζ_{15}	93.106192	.3508538	-.2013373	.0965502	-.0342052
ζ_{16}	49.032593	.2058541	-.0174195	-.0066318	.0032854
ζ_{17}	25.959773	.0427632	.3826631	-.2661559	.1020464
ζ_{18}	13.791156	.0021138	.5194669	-.4060948	.1578736
ζ_{19}	7.3420953	-.0001154	.1958513	.0473940	-.0416196
ζ_{20}	3.9136900	-.0000088	.0216982	.5616314	-.2904458
ζ_{21}	2.0876759	-.0001161	.0003773	.4638472	-.2918009
ζ_{22}	1.1140532	.0000586	.0008135	.1060160	.0897149
ζ_{23}	.59460959	-.0000413	-.0005313	.0104146	.4398681
ζ_{24}	.31739203	.0000244	.0003069	-.0008682	.4655616
ζ_{25}	.16942433	-.0000111	-.0001458	.0007707	.1742246
ζ_{26}	.09044012	.0000029	.0000408	-.0002847	.0338515

	Orbital	3d	4d		4f
	Energy	-35.89235	-4.78563		-0.54914
ζ_8	14128.469	.0000076	-.0000034		
ζ_9	6178.9780	.0000352	-.0000165		
ζ_{10}	2850.0951	.0001890	-.0000845		
ζ_{11}	1370.2289	.0008975	-.0004151		
ζ_{12}	679.78154	.0037663	-.0017137		
ζ_{13}	345.16717	.0145138	-.0067339	ζ_{13}	.0002706
ζ_{14}	178.21923	.0468358	-.0217450	ζ_{14}	.0008784
ζ_{15}	93.106192	.1265263	-.0602750	ζ_{15}	.0042670
ζ_{16}	49.032593	.2553315	-.1212660	ζ_{16}	.0154932
ζ_{17}	25.959773	.3604763	-.1650943	ζ_{17}	.0443189
ζ_{18}	13.791156	.2947997	-.0716395	ζ_{18}	.1062173
ζ_{19}	7.3420953	.1048229	.2136219	ζ_{19}	.1965545
ζ_{20}	3.9136900	.0140040	.4213015	ζ_{20}	.2652765
ζ_{21}	2.0876759	.0002217	.3602731	ζ_{21}	.2844776
ζ_{22}	1.1140532	.0002410	.1373398	ζ_{22}	.2353755
ζ_{23}	.59460959	-.0000622	.0295891	ζ_{23}	.1620190
ζ_{24}	.31739203			ζ_{24}	.0768975
ζ_{25}	.16942433			ζ_{25}	.0348289

Table 60-1. Nd ^{5}I (30s, 23p, 17d, 14f; 30 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	30	23	17	14
Nuclear charge	60	Number of closed shells	6	4	2	0
No. of electrons	60	Open-shell occupation	0	0	0	4

Coupling coefficients

$K_0^{ff} = -0.35714286$ $K_2^{ff} = -0.06746032$ $K_4^{ff} = -0.02912239$ $K_6^{ff} = -0.00334262$

Total energy	Potential energy	Kinetic energy	Virial theorem
-9283.882750	-18567.76680	9283.884060	-1.99999986

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1527.21285	-243.38435	-54.26314	-11.39573	-1.69816	-0.16578
ζ_1	83873014.	.0000015	-.0000005	.0000002	-.0000001	.0000000	.0000000
ζ_2	17257363.	.0000082	-.0000027	.0000012	-.0000006	.0000002	-.0000001
ζ_3	4096753.7	.0000460	-.0000151	.0000069	-.0000033	.0000013	-.0000003
ζ_4	1110803.4	.0002122	-.0000695	.0000317	-.0000150	.0000058	-.0000015
ζ_5	340029.45	.0008452	-.0002771	.0001265	-.0000598	.0000230	-.0000060
ζ_6	116011.80	.0029326	-.0009641	.0004404	-.0002086	.0000803	-.0000211
ζ_7	43520.584	.0090139	-.0029806	.0013616	-.0006439	.0002477	-.0000649
ζ_8	17705.576	.0247737	-.0083108	.0038080	-.0018056	.0006958	-.0001823
ζ_9	7707.7005	.0608542	-.0210400	.0096721	-.0045783	.0017611	-.0004613
ζ_{10}	3545.6406	.1311462	-.0482892	.0224402	-.0106813	.0041215	-.0010803
ζ_{11}	1704.1997	.2357752	-.0979392	.0462576	-.0220056	.0084684	-.0022183
ζ_{12}	847.51727	.3181383	-.1651756	.0810734	-.0391397	.0151654	-.0039778
ζ_{13}	432.52071	.2622369	-.1896717	.0984574	-.0476192	.0183376	-.0048027
ζ_{14}	225.00240	.0933993	-.0343525	.0201038	-.0110566	.0045843	-.0012180
ζ_{15}	118.68305	.0076559	.3582626	-.2657833	.1426032	-.0568484	.0149774
ζ_{16}	63.218006	.0006463	.5462182	-.5587098	.3134617	-.1242784	.0326705
ζ_{17}	33.901309	-.0003191	.2469016	-.2685414	.1844093	-.0798666	.0213146
ζ_{18}	18.261957	.0001426	.0251716	.6258689	-.5630621	.2564806	-.0688953
ζ_{19}	9.8661075	-.0001453	.0012706	.6723604	-.8830090	.4133422	-.1109441
ζ_{20}	5.3399625	.0001049	-.0005424	.1217496	.1634739	-.0935831	.0247601
ζ_{21}	2.8933981	-.0000695	.0000610	.0188010	.8758367	-.6456226	.1882509
ζ_{22}	1.5687454	.0000529	-.0001376	-.0075825	.4293851	-.5427909	.1671573
ζ_{23}	.85083575	-.0000382	.0000863	.0063881	.0237322	.2564459	-.0938315
ζ_{24}	.46154562	.0000270	-.0000493	-.0048943	.0137580	.7001385	-.2617637
ζ_{25}	.25039108	-.0000190	.0000379	.0034322	-.0075260	.4468025	-.3350252
ζ_{26}	.13584319	.0000128	-.0000241	-.0023697	.0056386	.0439141	-.1192152
ζ_{27}	.07369911	-.0000080	.0000151	.0014981	-.0035570	.0112884	.2527966
ζ_{28}	.03998419	.0000044	-.0000082	-.0008236	.0019738	-.0057899	.5642774
ζ_{29}	.02169275	-.0000018	.0000034	.0003451	-.0008325	.0025523	.3937257
ζ_{30}	.01176904	.0000004	-.0000008	-.0000802	.0001942	-.0006123	.0603461

Table 60-1. Nd ^{5}I (30s, 23p, 17d, 14f; 30 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-230.22585	-48.45457	-9.10847	-1.00583
ζ_5	340029.45	.0000041	-.0000020	.0000009	-.0000003
ζ_6	116011.80	.0000193	-.0000093	.0000043	-.0000015
ζ_7	43520.584	.0001032	-.0000495	.0000230	-.0000081
ζ_8	17705.576	.0004495	-.0002159	.0000998	-.0000349
ζ_9	7707.7005	.0017615	-.0008479	.0003945	-.0001384
ζ_{10}	3545.6406	.0061767	-.0029932	.0013874	-.0004852
ζ_{11}	1704.1997	.0195016	-.0095603	.0044627	-.0015664
ζ_{12}	847.51727	.0548843	-.0275465	.0128702	-.0045088
ζ_{13}	432.52071	.1325452	-.0691569	.0327145	-.0115114
ζ_{14}	225.00240	.2554914	-.1411621	.0673755	-.0237008
ζ_{15}	118.68305	.3477191	-.2035492	.0992396	-.0351555
ζ_{16}	63.218006	.2658731	-.1093889	.0450751	-.0152046
ζ_{17}	33.901309	.0855882	.2296285	-.1578985	.0591707
ζ_{18}	18.261957	.0075008	.5272650	-.4035895	.1571433
ζ_{19}	9.8661075	.0002971	.3318392	-.1900766	.0622612
ζ_{20}	5.3399625	-.0001692	.0587844	.3923527	-.1966264
ζ_{21}	2.8933981	-.0000362	.0058971	.5689440	-.3264583
ζ_{22}	1.5687454	-.0000215	-.0010896	.2483583	-.1189832
ζ_{23}	.85083575	.0000044	.0010578	.0290988	.2880675
ζ_{24}	.46154562	-.0000020	-.0007135	.0043069	.4802469
ζ_{25}	.25039108	.0000011	.0004080	-.0010892	.3465578
ζ_{26}	.13584319	-.0000005	-.0001848	.0005746	.0843712
ζ_{27}	.07369911	.0000001	.0000493	-.0002067	.0156926

	Orbital	3d	4d		4f
	Energy	-37.77263	-5.03593		-0.59575
ζ_8	17705.576	.0000051	-.0000023		
ζ_9	7707.7005	.0000235	-.0000109		
ζ_{10}	3545.6406	.0001278	-.0000584		
ζ_{11}	1704.1997	.0006084	-.0002806		
ζ_{12}	847.51727	.0025649	-.0011808		
ζ_{13}	432.52071	.0099918	-.0046408	ζ_{13}	.0001751
ζ_{14}	225.00240	.0331549	-.0154917	ζ_{14}	.0005740
ζ_{15}	118.68305	.0934660	-.0444598	ζ_{15}	.0027929
ζ_{16}	63.218006	.2058013	-.0990491	ζ_{16}	.0105481
ζ_{17}	33.901309	.3283229	-.1546624	ζ_{17}	.0320617
ζ_{18}	18.261957	.3374505	-.1303668	ζ_{18}	.0796146
ζ_{19}	9.8661075	.1720395	.0913532	ζ_{19}	.1618398
ζ_{20}	5.3399625	.0354749	.3565253	ζ_{20}	.2407249
ζ_{21}	2.8933981	.0025728	.4094097	ζ_{21}	.2783520
ζ_{22}	1.5687454	.0001325	.2331426	ζ_{22}	.2565648
ζ_{23}	.85083575	.0000379	.0617059	ζ_{23}	.1874586
ζ_{24}	.46154562	-.0000031	.0094410	ζ_{24}	.1128407
ζ_{25}	.25039108			ζ_{25}	.0463272
ζ_{26}	.13584319			ζ_{26}	.0151053

Table 60-2. Nd ^{5}I (29s, 22p, 16d, 13f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	29	22	16	13
Nuclear charge	60	Number of closed shells	6	4	2	0
No. of electrons	60	Open-shell occupation	0	0	0	4

Coupling coefficients

$K_0^{ff} = -0.35714286$ $K_2^{ff} = -0.06746032$ $K_4^{ff} = -0.02912239$ $K_6^{ff} = -0.00334262$

Total energy	Potential energy	Kinetic energy	Virial theorem
-9283.882591	-18567.76620	9283.883580	-1.99999990

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1527.21275	-243.38425	-54.26303	-11.39562	-1.69809	-0.16576
ζ_1	70882083.	.0000018	-.0000006	.0000003	-.0000001	.0000001	.0000000
ζ_2	14330165.	.0000104	-.0000034	.0000016	-.0000007	.0000003	-.0000001
ζ_3	3367158.5	.0000591	-.0000194	.0000088	-.0000042	.0000016	-.0000004
ζ_4	909197.80	.0002729	-.0000894	.0000408	-.0000193	.0000074	-.0000019
ζ_5	278458.67	.0010820	-.0003549	.0001620	-.0000767	.0000295	-.0000077
ζ_6	95349.961	.0037241	-.0012251	.0005593	-.0002648	.0001019	-.0000267
ζ_7	35955.746	.0113267	-.0037537	.0017166	-.0008124	.0003127	-.0000819
ζ_8	14706.564	.0307337	-.0103575	.0047446	-.0022484	.0008658	-.0002269
ζ_9	6430.2098	.0742084	-.0259411	.0119585	-.0056679	.0021825	-.0005718
ζ_{10}	2965.5246	.1556221	-.0585658	.0272630	-.0129706	.0049992	-.0013101
ζ_{11}	1425.6710	.2662074	-.1156911	.0551411	-.0263166	.0101486	-.0026591
ζ_{12}	707.34678	.3255615	-.1829848	.0907250	-.0438257	.0169484	-.0044442
ζ_{13}	359.23580	.2214112	-.1741967	.0932713	-.0455752	.0176635	-.0046295
ζ_{14}	185.53957	.0546346	.0676379	-.0437957	.0217520	-.0084542	.0022123
ζ_{15}	96.968358	.0025614	.4829124	-.3899352	.2117019	-.0839754	.0221040
ζ_{16}	51.090004	.0000540	.4892491	-.5693039	.3324953	-.1341452	.0353486
ζ_{17}	27.062917	.0000439	.1347396	.0473173	-.0257680	.0094624	-.0024177
ζ_{18}	14.385135	-.0001475	.0071529	.8250194	-.8661501	.4012204	-.1079152
ζ_{19}	7.6627515	.0000995	-.0002939	.4263039	-.5725056	.2686262	-.0721612
ζ_{20}	4.0870554	-.0000723	.0002599	.0398487	.6438937	-.3804654	.1048409
ζ_{21}	2.1814818	.0000598	-.0005106	.0053977	.7794779	-.7355614	.2236808
ζ_{22}	1.1648283	-.0000430	.0003590	-.0014571	.1611910	-.1825281	.0482494
ζ_{23}	.62209546	.0000306	-.0002625	.0009159	.0101785	.5878205	-.2001356
ζ_{24}	.33227001	-.0000217	.0001959	-.0007200	-.0010465	.6534546	-.3300869
ζ_{25}	.17747669	.0000146	-.0001316	.0004277	.0019384	.1801290	-.2569604
ζ_{26}	.09479758	-.0000092	.0000836	-.0002698	-.0011710	.0051664	.0947727
ζ_{27}	.05063547	.0000050	-.0000462	.0001467	.0006791	.0014969	.4940812
ζ_{28}	.02704661	-.0000021	.0000195	-.0000617	-.0002939	-.0005593	.5229989
ζ_{29}	.01444677	.0000005	-.0000046	.0000145	.0000702	.0001246	.1517253

Table 60-2. Nd ^{5}I (29s, 22p, 16d, 13f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-230.22575	-48.45446	-9.10836	-1.00577
ζ_5	278458.67	.0000058	-.0000028	.0000013	-.0000004
ζ_6	95349.961	.0000271	-.0000131	.0000061	-.0000021
ζ_7	35955.746	.0001430	-.0000683	.0000315	-.0000110
ζ_8	14706.564	.0006171	-.0002976	.0001385	-.0000486
ζ_9	6430.2098	.0023900	-.0011479	.0005312	-.0001857
ζ_{10}	2965.5246	.0083116	-.0040479	.0018862	-.0006618
ζ_{11}	1425.6710	.0259098	-.0127272	.0059212	-.0020727
ζ_{12}	707.34678	.0716841	-.0363790	.0170971	-.0060077
ζ_{13}	359.23580	.1664269	-.0878559	.0415205	-.0145798
ζ_{14}	185.53957	.2987825	-.1689924	.0814808	-.0287842
ζ_{15}	96.968358	.3511774	-.2024866	.0975065	-.0343173
ζ_{16}	51.090004	.2070921	-.0189946	-.0059118	.0030187
ζ_{17}	27.062917	.0432124	.3836844	-.2690014	.1025161
ζ_{18}	14.385135	.0021163	.5202799	-.4083967	.1576964
ζ_{19}	7.6627515	-.0001159	.1950577	.0519727	-.0435824
ζ_{20}	4.0870554	-.0000067	.0216058	.5633591	-.2895695
ζ_{21}	2.1814818	-.0001156	.0003278	.4609519	-.2871166
ζ_{22}	1.1648283	.0000592	.0008616	.1053231	.0887837
ζ_{23}	.62209546	-.0000416	-.0005569	.0103488	.4328969
ζ_{24}	.33227001	.0000246	.0003237	-.0008298	.4653779
ζ_{25}	.17747669	-.0000112	-.0001534	.0007625	.1795012
ζ_{26}	.09479758	.0000029	.0000427	-.0002789	.0358798

	Orbital	3d	4d		4f
	Energy	-37.77252	-5.03582		-0.59567
ζ_8	14706.564	.0000076	-.0000034		
ζ_9	6430.2098	.0000351	-.0000166		
ζ_{10}	2965.5246	.0001888	-.0000850		
ζ_{11}	1425.6710	.0008966	-.0004176		
ζ_{12}	707.34678	.0037651	-.0017250		
ζ_{13}	359.23580	.0145147	-.0067815	ζ_{13}	.0002828
ζ_{14}	185.53957	.0469023	-.0219319	ζ_{14}	.0009182
ζ_{15}	96.968358	.1268442	-.0608701	ζ_{15}	.0044669
ζ_{16}	51.090004	.2562539	-.1226319	ζ_{16}	.0162133
ζ_{17}	27.062917	.3614393	-.1666515	ζ_{17}	.0464245
ζ_{18}	14.385135	.2936139	-.0695836	ζ_{18}	.1108704
ζ_{19}	7.6627515	.1031766	.2189880	ζ_{19}	.2026875
ζ_{20}	4.0870554	.0136687	.4227520	ζ_{20}	.2696711
ζ_{21}	2.1814818	.0002528	.3565891	ζ_{21}	.2838612
ζ_{22}	1.1648283	.0002618	.1344541	ζ_{22}	.2304487
ζ_{23}	.62209546	-.0000537	.0289403	ζ_{23}	.1549211
ζ_{24}	.33227001			ζ_{24}	.0721882
ζ_{25}	.17747669			ζ_{25}	.0310353

Table 61-1. Pm ^{6}H (30s, 23p, 17d, 14f; 30 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	30	23	17	14
Nuclear charge	61	Number of closed shells	6	4	2	0
No. of electrons	61	Open-shell occupation	0	0	0	5

Coupling coefficients

$K_0^{ff} = -0.25714286$ $K_2^{ff} = -0.04368254$ $K_4^{ff} = -0.02515545$ $K_6^{ff} = -0.02292657$

Total energy	Potential energy	Kinetic energy	Virial theorem
-9655.098768	-19310.19930	9655.100520	-1.99999982

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1580.78955	-252.86123	-56.58309	-11.84813	-1.73935	-0.16759
ζ_1	87698351.	.0000015	-.0000005	.0000002	-.0000001	.0000000	.0000000
ζ_2	18083557.	.0000080	-.0000026	.0000012	-.0000006	.0000002	-.0000001
ζ_3	4298322.4	.0000452	-.0000148	.0000068	-.0000032	.0000012	-.0000003
ζ_4	1166063.4	.0002081	-.0000683	.0000313	-.0000148	.0000057	-.0000015
ζ_5	356926.50	.0008294	-.0002722	.0001246	-.0000591	.0000226	-.0000059
ζ_6	121723.04	.0028805	-.0009480	.0004342	-.0002062	.0000790	-.0000205
ζ_7	45633.356	.0088642	-.0029339	.0013441	-.0006374	.0002440	-.0000633
ζ_8	18552.126	.0243945	-.0081903	.0037634	-.0017891	.0006862	-.0001780
ζ_9	8071.2480	.0600139	-.0207591	.0095695	-.0045418	.0017388	-.0004509
ζ_{10}	3711.2577	.1295962	-.0477091	.0222311	-.0106096	.0040741	-.0010571
ζ_{11}	1783.4531	.2337431	-.0969506	.0459086	-.0218978	.0083872	-.0021751
ζ_{12}	886.99327	.3172918	-.1641352	.0807501	-.0390840	.0150703	-.0039129
ζ_{13}	452.81911	.2645970	-.1904297	.0990471	-.0480382	.0184149	-.0047751
ζ_{14}	235.69923	.0963025	-.0399239	.0233830	-.0127145	.0051980	-.0013636
ζ_{15}	124.42469	.0082086	.3500571	-.2595704	.1396189	-.0553866	.0144422
ζ_{16}	66.341243	.0006736	.5479880	-.5590386	.3145176	-.1241366	.0323093
ζ_{17}	35.616113	-.0003353	.2543968	-.2834583	.1941228	-.0833520	.0219922
ζ_{18}	19.209335	.0001584	.0267828	.6153372	-.5544326	.2510872	-.0667160
ζ_{19}	10.391565	-.0001588	.0013660	.6820097	-.8926463	.4159582	-.1105289
ζ_{20}	5.6320715	.0001151	-.0005939	.1276206	.1461126	-.0847937	.0222642
ζ_{21}	3.0559745	-.0000771	.0001089	.0192433	.8720086	-.6329852	.1818214
ζ_{22}	1.6592671	.0000588	-.0001759	-.0075646	.4418716	-.5484480	.1672554
ζ_{23}	.90123566	-.0000426	.0001137	.0064397	.0266865	.2302102	-.0839858
ζ_{24}	.48959815	.0000302	-.0000691	-.0049351	.0140909	.6877296	-.2502584
ζ_{25}	.26599802	-.0000214	.0000516	.0034673	-.0077032	.4659631	-.3299549
ζ_{26}	.14452159	.0000144	-.0000330	-.0023977	.0058056	.0536079	-.1364816
ζ_{27}	.07852226	-.0000091	.0000205	.0015167	-.0036627	.0112461	.2237586
ζ_{28}	.04266332	.0000050	-.0000110	-.0008338	.0020329	-.0055822	.5485797
ζ_{29}	.02318018	-.0000021	.0000046	.0003492	-.0008568	.0024730	.4207136
ζ_{30}	.01259445	.0000005	-.0000010	-.0000810	.0001996	-.0005943	.0776294

Table 61-1. Pm ^{6}H (30s, 23p, 17d, 14f; 30 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-239.43783	-50.63174	-9.49063	-1.02724
ζ_5	356926.50	.0000040	-.0000019	.0000009	-.0000003
ζ_6	121723.04	.0000189	-.0000091	.0000042	-.0000015
ζ_7	45633.356	.0001010	-.0000486	.0000227	-.0000079
ζ_8	18552.126	.0004403	-.0002122	.0000984	-.0000341
ζ_9	8071.2480	.0017276	-.0008346	.0003896	-.0001358
ζ_{10}	3711.2577	.0060638	-.0029486	.0013711	-.0004762
ζ_{11}	1783.4531	.0191673	-.0094292	.0044163	-.0015396
ζ_{12}	886.99327	.0540097	-.0271949	.0127470	-.0044355
ζ_{13}	452.81911	.1307405	-.0684320	.0324807	-.0113519
ζ_{14}	235.69923	.2530244	-.1402136	.0671435	-.0234601
ζ_{15}	124.42469	.3469600	-.2039126	.0997885	-.0351130
ζ_{16}	66.341243	.2688423	-.1137184	.0476140	-.0160134
ζ_{17}	35.616113	.0883136	.2234379	-.1549596	.0577183
ζ_{18}	19.209335	.0079311	.5268490	-.4048125	.1565308
ζ_{19}	10.391565	.0003206	.3368634	-.1964217	.0645601
ζ_{20}	5.6320715	-.0001785	.0608837	.3866839	-.1928416
ζ_{21}	3.0559745	-.0000272	.0061353	.5691699	-.3224459
ζ_{22}	1.6592671	-.0000281	-.0010940	.2540310	-.1245540
ζ_{23}	.90123566	.0000089	.0010887	.0307557	.2751435
ζ_{24}	.48959815	-.0000049	-.0007301	.0045327	.4732285
ζ_{25}	.26599802	.0000028	.0004181	-.0011264	.3569230
ζ_{26}	.14452159	-.0000012	-.0001894	.0006100	.0927525
ζ_{27}	.07852226	.0000003	.0000504	-.0002156	.0175195

	Orbital	3d	4d		4f
	Energy	-39.68738	-5.28715		-0.62826
ζ_8	18552.126	.0000050	-.0000023		
ζ_9	8071.2480	.0000231	-.0000108		
ζ_{10}	3711.2577	.0001258	-.0000579		
ζ_{11}	1783.4531	.0005992	-.0002780		
ζ_{12}	886.99327	.0025282	-.0011712		
ζ_{13}	452.81911	.0098525	-.0046042	ζ_{13}	.0001786
ζ_{14}	235.69923	.0327518	-.0154007	ζ_{14}	.0005855
ζ_{15}	124.42469	.0925319	-.0442930	ζ_{15}	.0028532
ζ_{16}	66.341243	.2045131	-.0991045	ζ_{16}	.0107807
ζ_{17}	35.616113	.3277010	-.1555263	ζ_{17}	.0328565
ζ_{18}	19.209335	.3381709	-.1317159	ζ_{18}	.0816076
ζ_{19}	10.391565	.1732506	.0905880	ζ_{19}	.1649973
ζ_{20}	5.6320715	.0360085	.3560379	ζ_{20}	.2434446
ζ_{21}	3.0559745	.0027124	.4085786	ζ_{21}	.2785354
ζ_{22}	1.6592671	.0001642	.2340863	ζ_{22}	.2540409
ζ_{23}	.90123566	.0000519	.0625248	ζ_{23}	.1839785
ζ_{24}	.48959815	.0000004	.0098761	ζ_{24}	.1101246
ζ_{25}	.26599802			ζ_{25}	.0451532
ζ_{26}	.14452159			ζ_{26}	.0147935

Table 61-2. Pm ^{6}H (29s, 22p, 16d, 13f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	29	22	16	13
Nuclear charge	61	Number of closed shells	6	4	2	0
No. of electrons	61	Open-shell occupation	0	0	0	5

Coupling coefficients

$K_0^{ff} = -0.25714286$ $K_2^{ff} = -0.04368254$ $K_4^{ff} = -0.02515545$ $K_6^{ff} = -0.02292657$

Total energy	Potential energy	Kinetic energy	Virial theorem
-9655.098597	-19310.19870	9655.100090	-1.99999985

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1580.78944	-252.86112	-56.58298	-11.84802	-1.73928	-0.16757
ζ_1	73792259.	.0000018	-.0000006	.0000003	-.0000001	.0000000	.0000000
ζ_2	14912669.	.0000103	-.0000034	.0000015	-.0000007	.0000003	-.0000001
ζ_3	3503063.3	.0000587	-.0000192	.0000088	-.0000042	.0000016	-.0000004
ζ_4	945733.66	.0002708	-.0000888	.0000406	-.0000193	.0000074	-.0000019
ζ_5	289625.72	.0010738	-.0003526	.0001615	-.0000766	.0000293	-.0000076
ζ_6	99173.521	.0036957	-.0012170	.0005572	-.0002645	.0001013	-.0000263
ζ_7	37399.674	.0112400	-.0037289	.0017101	-.0008115	.0003109	-.0000806
ζ_8	15298.651	.0305010	-.0102890	.0047266	-.0022457	.0008607	-.0002232
ζ_9	6689.9213	.0736733	-.0257733	.0119152	-.0056626	.0021701	-.0005628
ζ_{10}	3085.7259	.1546490	-.0582207	.0271774	-.0129640	.0049727	-.0012901
ζ_{11}	1483.6688	.2650880	-.1151508	.0550385	-.0263395	.0101095	-.0026222
ζ_{12}	736.22554	.3255532	-.1826711	.0908042	-.0439798	.0169263	-.0043937
ζ_{13}	373.95246	.2231210	-.1753525	.0941539	-.0461461	.0178027	-.0046191
ζ_{14}	193.16494	.0558003	.0641484	-.0418187	.0208364	-.0080642	.0020886
ζ_{15}	100.96558	.0026327	.4807420	-.3888686	.2117416	-.0835864	.0217796
ζ_{16}	53.201961	.0000743	.4921413	-.5741796	.3368415	-.1353240	.0352985
ζ_{17}	28.184615	.0000289	.1366487	.0447115	-.0249484	.0092146	-.0023306
ζ_{18}	14.982875	-.0001359	.0071619	.8282511	-.8746845	.4032216	-.1073254
ζ_{19}	7.9819341	.0000912	-.0002585	.4261629	-.5690547	.2656068	-.0705824
ζ_{20}	4.2576997	-.0000662	.0002371	.0398653	.6494843	-.3829024	.1043786
ζ_{21}	2.2727753	.0000553	-.0004910	.0051980	.7757111	-.7276966	.2185475
ζ_{22}	1.2136872	-.0000397	.0003465	-.0013150	.1604693	-.1805365	.0475640
ζ_{23}	.64824860	.0000283	-.0002539	.0008155	.0100618	.5780210	-.1939498
ζ_{24}	.34627032	-.0000201	.0001899	-.0006430	-.0009643	.6526874	-.3227025
ζ_{25}	.18497156	.0000135	-.0001275	.0003754	.0018766	.1862266	-.2572668
ζ_{26}	.09880988	-.0000085	.0000811	-.0002365	-.0011278	.0055972	.0808819
ζ_{27}	.05278341	.0000047	-.0000448	.0001282	.0006548	.0016596	.4817937
ζ_{28}	.02819648	-.0000020	.0000189	-.0000539	-.0002834	-.0006319	.5269040
ζ_{29}	.01506233	.0000005	-.0000045	.0000127	.0000677	.0001423	.1673525

Table 61-2. Pm ^{6}H (29s, 22p, 16d, 13f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-239.43773	-50.63163	-9.49052	-1.02717
ζ_5	289625.72	.0000058	-.0000028	.0000013	-.0000004
ζ_6	99173.521	.0000269	-.0000130	.0000061	-.0000021
ζ_7	37399.674	.0001418	-.0000679	.0000314	-.0000109
ζ_8	15298.651	.0006115	-.0002960	.0001382	-.0000482
ζ_9	6689.9213	.0023683	-.0011415	.0005300	-.0001840
ζ_{10}	3085.7259	.0082371	-.0040261	.0018824	-.0006560
ζ_{11}	1483.6688	.0256921	-.0126649	.0059113	-.0020552
ζ_{12}	736.22554	.0711525	-.0362370	.0170886	-.0059643
ζ_{13}	373.95246	.1655104	-.0876824	.0415779	-.0145017
ζ_{14}	193.16494	.2979782	-.1691667	.0818614	-.0287250
ζ_{15}	100.96558	.3516814	-.2037196	.0984695	-.0344267
ζ_{16}	53.201961	.2084724	-.0206403	-.0051412	.0027340
ζ_{17}	28.184615	.0436458	.3850121	-.2719277	.1029987
ζ_{18}	14.982875	.0021159	.5212128	-.4105337	.1574192
ζ_{19}	7.9819341	-.0001187	.1939588	.0572835	-.0458037
ζ_{20}	4.2576997	-.0000027	.0214107	.5656179	-.2889627
ζ_{21}	2.2727753	-.0001164	.0002716	.4575787	-.2822454
ζ_{22}	1.2136872	.0000608	.0009081	.1040554	.0891011
ζ_{23}	.64824860	-.0000425	-.0005826	.0102158	.4274215
ζ_{24}	.34627032	.0000251	.0003404	-.0008080	.4645273
ζ_{25}	.18497156	-.0000114	-.0001610	.0007575	.1834688
ζ_{26}	.09880988	.0000030	.0000447	-.0002741	.0374927

	Orbital	3d	4d		4f
	Energy	-39.68727	-5.28704		-0.62818
ζ_8	15298.651	.0000076	-.0000034		
ζ_9	6689.9213	.0000350	-.0000167		
ζ_{10}	3085.7259	.0001882	-.0000852		
ζ_{11}	1483.6688	.0008937	-.0004189		
ζ_{12}	736.22554	.0037555	-.0017312		
ζ_{13}	373.95246	.0144900	-.0068130	ζ_{13}	.0002930
ζ_{14}	193.16494	.0469140	-.0220785	ζ_{14}	.0009524
ζ_{15}	100.96558	.1271069	-.0614014	ζ_{15}	.0046428
ζ_{16}	53.201961	.2572321	-.1239514	ζ_{16}	.0168607
ζ_{17}	28.184615	.3625802	-.1681830	ζ_{17}	.0483640
ζ_{18}	14.982875	.2925031	-.0673861	ζ_{18}	.1151252
ζ_{19}	7.9819341	.1014651	.2245593	ζ_{19}	.2080499
ζ_{20}	4.2576997	.0133021	.4243576	ζ_{20}	.2729885
ζ_{21}	2.2727753	.0002779	.3528129	ζ_{21}	.2826146
ζ_{22}	1.2136872	.0002809	.1313945	ζ_{22}	.2258746
ζ_{23}	.64824860	-.0000460	.0281380	ζ_{23}	.1494945
ζ_{24}	.34627032			ζ_{24}	.0688871
ζ_{25}	.18497156			ζ_{25}	.0289222

Table 62-1. Sm ^{7}F (30s, 23p, 17d, 14f; 30 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	30	23	17	14
Nuclear charge	62	Number of closed shells	6	4	2	0
No. of electrons	62	Open-shell occupation	0	0	0	6

Coupling coefficients

$K_0^{ff} = -0.19047619$ $K_2^{ff} = -0.03597884$ $K_4^{ff} = -0.02453102$ $K_6^{ff} = -0.03145003$

Total energy	Potential energy	Kinetic energy	Virial theorem
-10034.95234	-20069.90690	10034.95460	-1.99999977

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1635.28439	-262.50537	-58.93295	-12.29796	-1.77865	-0.16931
ζ_1	91563325.	.0000014	-.0000005	.0000002	-.0000001	.0000000	.0000000
ζ_2	18870699.	.0000079	-.0000026	.0000012	-.0000006	.0000002	-.0000001
ζ_3	4483943.3	.0000446	-.0000147	.0000067	-.0000032	.0000012	-.0000003
ζ_4	1216216.8	.0002057	-.0000675	.0000310	-.0000148	.0000056	-.0000014
ζ_5	372264.81	.0008197	-.0002693	.0001236	-.0000587	.0000224	-.0000058
ζ_6	126961.41	.0028464	-.0009377	.0004307	-.0002050	.0000782	-.0000201
ζ_7	47602.898	.0087586	-.0029019	.0013330	-.0006335	.0002413	-.0000620
ζ_8	19355.702	.0241062	-.0081007	.0037322	-.0017783	.0006785	-.0001744
ζ_9	8422.1037	.0593347	-.0205364	.0094924	-.0045154	.0017197	-.0004419
ζ_{10}	3873.0847	.1282959	-.0472334	.0220669	-.0105551	.0040322	-.0010365
ζ_{11}	1861.3964	.2320270	-.0961409	.0456410	-.0218193	.0083142	-.0021362
ζ_{12}	925.80775	.3166303	-.1633405	.0805425	-.0390715	.0149868	-.0038550
ζ_{13}	472.63914	.2666074	-.1911536	.0996453	-.0484427	.0184769	-.0047471
ζ_{14}	246.00813	.0986284	-.0441090	.0258403	-.0139732	.0056518	-.0014667
ζ_{15}	129.85778	.0086206	.3448957	-.2559391	.1380061	-.0544590	.0140662
ζ_{16}	69.231135	.0006968	.5498955	-.5611563	.3166187	-.1243620	.0320705
ζ_{17}	37.162905	-.0003517	.2589082	-.2916198	.1998749	-.0852056	.0222546
ζ_{18}	20.040665	.0001735	.0274559	.6146329	-.5569671	.2508545	-.0659965
ζ_{19}	10.839544	-.0001707	.0014378	.6854973	-.8972532	.4159543	-.1094881
ζ_{20}	5.8738649	.0001243	-.0006519	.1284519	.1490520	-.0865396	.0226065
ζ_{21}	3.1866043	-.0000841	.0001597	.0192909	.8709301	-.6276879	.1781235
ζ_{22}	1.7298774	.0000639	-.0002125	-.0075829	.4416251	-.5431837	.1640059
ζ_{23}	.93941350	-.0000462	.0001409	.0064609	.0271244	.2221911	-.0800608
ζ_{24}	.51024282	.0000328	-.0000889	-.0049440	.0140174	.6798195	-.2433364
ζ_{25}	.27716212	-.0000232	.0000655	.0034756	-.0076627	.4717147	-.3247542
ζ_{26}	.15055888	.0000156	-.0000424	-.0024034	.0057866	.0580159	-.1430275
ζ_{27}	.08178705	-.0000098	.0000263	.0015203	-.0036509	.0111096	.2095432
ζ_{28}	.04442878	.0000054	-.0000142	-.0008359	.0020272	-.0054160	.5391598
ζ_{29}	.02413486	-.0000023	.0000059	.0003501	-.0008546	.0024071	.4323881
ζ_{30}	.01311067	.0000005	-.0000014	-.0000812	.0001992	-.0005796	.0873294

Table 62-1. Sm ^{7}F (30s, 23p, 17d, 14f; 30 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-248.81712	-52.83841	-9.87003	-1.04713
ζ_5	372264.81	.0000040	-.0000019	.0000009	-.0000003
ζ_6	126961.41	.0000186	-.0000090	.0000042	-.0000014
ζ_7	47602.898	.0000995	-.0000480	.0000225	-.0000078
ζ_8	19355.702	.0004336	-.0002097	.0000975	-.0000336
ζ_9	8422.1037	.0017014	-.0008247	.0003861	-.0001336
ζ_{10}	3873.0847	.0059734	-.0029146	.0013591	-.0004687
ζ_{11}	1861.3964	.0188979	-.0093272	.0043809	-.0015162
ζ_{12}	925.80775	.0533264	-.0269377	.0126624	-.0043743
ζ_{13}	472.63914	.1294294	-.0679553	.0323471	-.0112230
ζ_{14}	246.00813	.2514824	-.1398040	.0671471	-.0232933
ζ_{15}	129.85778	.3468742	-.2046208	.1004496	-.0350887
ζ_{16}	69.231135	.2709646	-.1165381	.0492792	-.0164934
ζ_{17}	37.162905	.0897984	.2217687	-.1549571	.0573527
ζ_{18}	20.040665	.0080848	.5284040	-.4078800	.1565510
ζ_{19}	10.839544	.0003313	.3376618	-.1959364	.0638163
ζ_{20}	5.8738649	-.0001862	.0608114	.3896261	-.1930263
ζ_{21}	3.1866043	-.0000190	.0061322	.5680084	-.3187796
ζ_{22}	1.7298774	-.0000327	-.0010838	.2528972	-.1226721
ζ_{23}	.93941350	.0000123	.0010906	.0306572	.2707020
ζ_{24}	.51024282	-.0000071	-.0007276	.0045142	.4686257
ζ_{25}	.27716212	.0000040	.0004171	-.0011131	.3600954
ζ_{26}	.15055888	-.0000017	-.0001890	.0006101	.0965668
ζ_{27}	.08178705	.0000004	.0000503	-.0002140	.0183374

	Orbital	3d	4d		4f
	Energy	-41.63097	-5.53537		-0.66637
ζ_8	19355.702	.0000049	-.0000023		
ζ_9	8422.1037	.0000229	-.0000107		
ζ_{10}	3873.0847	.0001244	-.0000575		
ζ_{11}	1861.3964	.0005927	-.0002765		
ζ_{12}	925.80775	.0025022	-.0011653		
ζ_{13}	472.63914	.0097667	-.0045897	ζ_{13}	.0001827
ζ_{14}	246.00813	.0325495	-.0153900	ζ_{14}	.0006008
ζ_{15}	129.85778	.0922524	-.0444142	ζ_{15}	.0029328
ζ_{16}	69.231135	.2045770	-.0997265	ζ_{16}	.0111103
ζ_{17}	37.162905	.3286497	-.1569771	ζ_{17}	.0339508
ζ_{18}	20.040665	.3385538	-.1319127	ζ_{18}	.0844008
ζ_{19}	10.839544	.1722616	.0939747	ζ_{19}	.1694842
ζ_{20}	5.8738649	.0354474	.3591156	ζ_{20}	.2474187
ζ_{21}	3.1866043	.0027003	.4071765	ζ_{21}	.2794933
ζ_{22}	1.7298774	.0001947	.2312748	ζ_{22}	.2512643
ζ_{23}	.93941350	.0000602	.0612840	ζ_{23}	.1795363
ζ_{24}	.51024282	.0000044	.0097258	ζ_{24}	.1057905
ζ_{25}	.27716212			ζ_{25}	.0427739
ζ_{26}	.15055888			ζ_{26}	.0135339

Table 62-2. Sm ^{7}F (29s, 22p, 16d, 13f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	29	22	16	13
Nuclear charge	62	Number of closed shells	6	4	2	0
No. of electrons	62	Open-shell occupation	0	0	0	6

Coupling coefficients

$K_0^{ff} = -0.19047619$ $K_2^{ff} = -0.03597884$ $K_4^{ff} = -0.02453102$ $K_6^{ff} = -0.03145003$

Total energy	Potential energy	Kinetic energy	Virial theorem
-10034.95216	-20069.90580	10034.95360	-1.99999986

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1635.28430	-262.50528	-58.93286	-12.29786	-1.77859	-0.16929
ζ_1	76599430.	.0000018	-.0000006	.0000003	-.0000001	.0000000	.0000000
ζ_2	15436757.	.0000103	-.0000034	.0000016	-.0000007	.0000003	-.0000001
ζ_3	3619392.3	.0000587	-.0000193	.0000088	-.0000042	.0000016	-.0000004
ζ_4	976104.90	.0002713	-.0000891	.0000409	-.0000194	.0000074	-.0000019
ζ_5	298812.85	.0010758	-.0003536	.0001624	-.0000772	.0000294	-.0000076
ζ_6	102334.40	.0037002	-.0012199	.0005600	-.0002664	.0001016	-.0000261
ζ_7	38611.783	.0112422	-.0037337	.0017170	-.0008166	.0003113	-.0000800
ζ_8	15806.320	.0304719	-.0102906	.0047401	-.0022572	.0008606	-.0002212
ζ_9	6917.8249	.0735253	-.0257492	.0119375	-.0056864	.0021681	-.0005571
ζ_{10}	3193.5967	.1542399	-.0581236	.0272058	-.0130067	.0049632	-.0012757
ζ_{11}	1536.7667	.2644285	-.1149371	.0550947	-.0264300	.0100925	-.0025935
ζ_{12}	763.10995	.3252931	-.1825171	.0909726	-.0441615	.0169075	-.0043482
ζ_{13}	387.83565	.2238872	-.1759510	.0947753	-.0465814	.0178820	-.0045966
ζ_{14}	200.43085	.0564499	.0622804	-.0408836	.0204526	-.0078826	.0020224
ζ_{15}	104.80186	.0026716	.4796447	-.3890638	.2124092	-.0834094	.0215312
ζ_{16}	55.238792	.0000876	.4938579	-.5782957	.3407802	-.1362871	.0352183
ζ_{17}	29.269732	.0000182	.1375698	.0454653	-.0266296	.0100369	-.0025257
ζ_{18}	15.562115	-.0001271	.0070940	.8318606	-.8840923	.4054264	-.1068752
ζ_{19}	8.2914716	.0000850	-.0002319	.4239646	-.5619932	.2607135	-.0685858
ζ_{20}	4.4232048	-.0000616	.0002194	.0396437	.6563798	-.3859066	.1041507
ζ_{21}	2.3612917	.0000519	-.0004738	.0048858	.7706911	-.7190816	.2135060
ζ_{22}	1.2610331	-.0000372	.0003358	-.0010984	.1589026	-.1773998	.0465316
ζ_{23}	.67357403	.0000266	-.0002465	.0006583	.0099796	.5689596	-.1883146
ζ_{24}	.35981703	-.0000189	.0001846	-.0005253	-.0009516	.6513834	-.3160327
ζ_{25}	.19221775	.0000126	-.0001240	.0002953	.0018588	.1916307	-.2568383
ζ_{26}	.10268588	-.0000079	.0000789	-.0001856	-.0011136	.0060965	.0683084
ζ_{27}	.05485668	.0000044	-.0000435	.0001000	.0006468	.0017746	.4708873
ζ_{28}	.02930547	-.0000018	.0000184	-.0000419	-.0002799	-.0006838	.5288893
ζ_{29}	.01565553	.0000004	-.0000043	.0000098	.0000669	.0001551	.1824843

Table 62-2. Sm ^{7}F (29s, 22p, 16d, 13f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-248.81704	-52.83832	-9.86992	-1.04707
ζ_5	298812.85	.0000058	-.0000028	.0000013	-.0000004
ζ_6	102334.40	.0000270	-.0000131	.0000061	-.0000021
ζ_7	38611.783	.0001421	-.0000683	.0000317	-.0000109
ζ_8	15806.320	.0006120	-.0002973	.0001392	-.0000482
ζ_9	6917.8249	.0023668	-.0011447	.0005329	-.0001837
ζ_{10}	3193.5967	.0082210	-.0040323	.0018909	-.0006542
ζ_{11}	1536.7667	.0256204	-.0126733	.0059316	-.0020473
ζ_{12}	763.10995	.0709298	-.0362523	.0171477	-.0059418
ζ_{13}	387.83565	.1650761	-.0877685	.0417403	-.0144532
ζ_{14}	200.43085	.2975720	-.1695881	.0823343	-.0286841
ζ_{15}	104.80186	.3519038	-.2046806	.0992392	-.0344467
ζ_{16}	55.238792	.2090819	-.0211105	-.0050311	.0026864
ζ_{17}	29.269732	.0437401	.3874871	-.2756017	.1037013
ζ_{18}	15.562115	.0020934	.5214855	-.4118324	.1567035
ζ_{19}	8.2914716	-.0001230	.1919297	.0642447	-.0486498
ζ_{20}	4.4232048	.0000021	.0210959	.5679134	-.2881766
ζ_{21}	2.3612917	-.0001173	.0001901	.4534835	-.2769052
ζ_{22}	1.2610331	.0000624	.0009669	.1024279	.0898095
ζ_{23}	.67357403	-.0000435	-.0006172	.0100632	.4222292
ζ_{24}	.35981703	.0000257	.0003623	-.0008015	.4634404
ζ_{25}	.19221775	-.0000117	-.0001710	.0007567	.1870819
ζ_{26}	.10268588	.0000030	.0000472	-.0002708	.0390885

	Orbital	3d	4d		4f
	Energy	-41.63088	-5.53527		-0.66629
ζ_8	15806.320	.0000077	-.0000035		
ζ_9	6917.8249	.0000352	-.0000169		
ζ_{10}	3193.5967	.0001895	-.0000862		
ζ_{11}	1536.7667	.0008976	-.0004230		
ζ_{12}	763.10995	.0037700	-.0017473		
ζ_{13}	387.83565	.0145380	-.0068741	ζ_{13}	.0003049
ζ_{14}	200.43085	.0471074	-.0222968	ζ_{14}	.0009896
ζ_{15}	104.80186	.1277149	-.0620623	ζ_{15}	.0048333
ζ_{16}	55.238792	.2585899	-.1253644	ζ_{16}	.0175402
ζ_{17}	29.269732	.3637340	-.1695404	ζ_{17}	.0503597
ζ_{18}	15.562115	.2908504	-.0644996	ζ_{18}	.1194008
ζ_{19}	8.2914716	.0993883	.2305640	ζ_{19}	.2132458
ζ_{20}	4.4232048	.0128814	.4257140	ζ_{20}	.2760468
ζ_{21}	2.3612917	.0002968	.3487330	ζ_{21}	.2812882
ζ_{22}	1.2610331	.0002992	.1282967	ζ_{22}	.2214440
ζ_{23}	.67357403	-.0000397	.0273106	ζ_{23}	.1441161
ζ_{24}	.35981703			ζ_{24}	.0655359
ζ_{25}	.19221775			ζ_{25}	.0266061

Table 63-1. Eu ^{8}S (30s, 23p, 17d, 14f; 30 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	30	23	17	14
Nuclear charge	63	Number of closed shells	6	4	2	0
No. of electrons	63	Open-shell occupation	0	0	0	7

Coupling coefficients

$K_0^{ff} = -0.14285714$ $K_2^{ff} = -0.03809524$ $K_4^{ff} = -0.02597403$ $K_6^{ff} = -0.03330003$

Total energy	Potential energy	Kinetic energy	Virial theorem
-10423.54280	-20847.08840	10423.54560	-1.99999973

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1690.69637	-272.31573	-61.31187	-12.74470	-1.81600	-0.17096
ζ_1	95573524.	.0000014	-.0000005	.0000002	-.0000001	.0000000	.0000000
ζ_2	19684999.	.0000078	-.0000026	.0000012	-.0000006	.0000002	-.0000001
ζ_3	4675605.5	.0000441	-.0000145	.0000067	-.0000032	.0000012	-.0000003
ζ_4	1267953.8	.0002033	-.0000668	.0000308	-.0000147	.0000056	-.0000014
ζ_5	388084.60	.0008100	-.0002664	.0001226	-.0000584	.0000221	-.0000056
ζ_6	132366.25	.0028124	-.0009275	.0004271	-.0002037	.0000772	-.0000197
ζ_7	49636.469	.0086530	-.0028697	.0013216	-.0006293	.0002384	-.0000607
ζ_8	20186.104	.0238169	-.0080103	.0037000	-.0017664	.0006702	-.0001708
ζ_9	8784.9681	.0586504	-.0203110	.0094122	-.0044857	.0016990	-.0004328
ζ_{10}	4040.5623	.1269796	-.0467497	.0218951	-.0104930	.0039861	-.0010160
ζ_{11}	1942.0969	.2302750	-.0953124	.0453566	-.0217245	.0082321	-.0020972
ζ_{12}	966.00250	.3159214	-.1625102	.0803045	-.0390299	.0148865	-.0037964
ζ_{13}	493.16211	.2686230	-.1918415	.1002093	-.0488136	.0185173	-.0047174
ζ_{14}	256.67894	.1010269	-.0483378	.0283290	-.0152474	.0061039	-.0015686
ζ_{15}	135.47839	.0090608	.3395501	-.2521082	.1362201	-.0534482	.0136854
ζ_{16}	72.218462	.0007200	.5517414	-.5630350	.3184438	-.1244163	.0318141
ζ_{17}	38.760363	-.0003677	.2635652	-.3000220	.2056841	-.0870123	.0225153
ζ_{18}	20.898321	.0001885	.0281806	.6133672	-.5585150	.2500236	-.0651787
ζ_{19}	11.301178	-.0001827	.0015127	.6892240	-.9015651	.4155665	-.1084389
ζ_{20}	6.1227230	.0001335	-.0007101	.1294894	.1505741	-.0874551	.0227342
ζ_{21}	3.3208792	-.0000911	.0002113	.0193593	.8693310	-.6211022	.1742400
ζ_{22}	1.8023626	.0000690	-.0002501	-.0076003	.4423072	-.5387141	.1611776
ζ_{23}	.97855234	-.0000500	.0001689	.0064840	.0276955	.2127537	-.0758468
ζ_{24}	.53137824	.0000356	-.0001095	-.0049543	.0139867	.6716246	-.2366260
ζ_{25}	.28857580	-.0000251	.0000800	.0034846	-.0076527	.4781292	-.3198590
ζ_{26}	.15672251	.0000170	-.0000522	-.0024095	.0057901	.0629254	-.1494450
ζ_{27}	.08511546	-.0000107	.0000326	.0015241	-.0036535	.0109867	.1953804
ζ_{28}	.04622609	.0000058	-.0000177	-.0008381	.0020295	-.0052362	.5296623
ζ_{29}	.02510535	-.0000024	.0000073	.0003511	-.0008559	.0023355	.4431703
ζ_{30}	.01363470	.0000006	-.0000017	-.0000815	.0001995	-.0005634	.0977662

Table 63-1. Eu ^{8}S (30s, 23p, 17d, 14f; 30 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-258.36268	-55.07373	-10.24610	-1.06546
ζ_5	388084.60	.0000039	-.0000019	.0000009	-.0000003
ζ_6	132366.25	.0000183	-.0000089	.0000041	-.0000014
ζ_7	49636.469	.0000980	-.0000474	.0000223	-.0000076
ζ_8	20186.104	.0004269	-.0002071	.0000965	-.0000330
ζ_9	8784.9681	.0016751	-.0008145	.0003823	-.0001312
ζ_{10}	4040.5623	.0058821	-.0028793	.0013459	-.0004605
ζ_{11}	1942.0969	.0186250	-.0092212	.0043416	-.0014909
ζ_{12}	966.00250	.0526313	-.0266679	.0125659	-.0043075
ζ_{13}	493.16211	.1280877	-.0674470	.0321839	-.0110797
ζ_{14}	256.67894	.2498856	-.1393310	.0670893	-.0230945
ζ_{15}	135.47839	.3467539	-.2052730	.1010429	-.0350217
ζ_{16}	72.218462	.2731421	-.1194207	.0509718	-.0169671
ζ_{17}	38.760363	.0913547	.2198456	-.1546832	.0568534
ζ_{18}	20.898321	.0082541	.5298352	-.4105853	.1563290
ζ_{19}	11.301178	.0003434	.3386907	-.1957815	.0632035
ζ_{20}	6.1227230	-.0001939	.0608493	.3917558	-.1926379
ζ_{21}	3.3208792	-.0000106	.0061453	.5668611	-.3148090
ζ_{22}	1.8023626	-.0000375	-.0010767	.2523752	-.1215365
ζ_{23}	.97855234	.0000159	.0010954	.0306878	.2655109
ζ_{24}	.53137824	-.0000094	-.0007272	.0045182	.4638945
ζ_{25}	.28857580	.0000053	.0004173	-.0011102	.3637009
ζ_{26}	.15672251	-.0000023	-.0001892	.0006148	.1008133
ζ_{27}	.08511546	.0000006	.0000503	-.0002138	.0192946

	Orbital	3d	4d		4f
	Energy	-43.60249	-5.77998		-0.71167
ζ_8	20186.104	.0000048	-.0000022		
ζ_9	8784.9681	.0000226	-.0000106		
ζ_{10}	4040.5623	.0001228	-.0000570		
ζ_{11}	1942.0969	.0005857	-.0002746		
ζ_{12}	966.00250	.0024743	-.0011577		
ζ_{13}	493.16211	.0096736	-.0045682	ζ_{13}	.0001861
ζ_{14}	256.67894	.0323236	-.0153573	ζ_{14}	.0006141
ζ_{15}	135.47839	.0919099	-.0444727	ζ_{15}	.0030038
ζ_{16}	72.218462	.2045360	-.1002326	ζ_{16}	.0114090
ζ_{17}	38.760363	.3294971	-.1582806	ζ_{17}	.0349642
ζ_{18}	20.898321	.3389885	-.1321230	ζ_{18}	.0869983
ζ_{19}	11.301178	.1714660	.0969335	ζ_{19}	.1736389
ζ_{20}	6.1227230	.0349844	.3616452	ζ_{20}	.2510775
ζ_{21}	3.3208792	.0027018	.4058108	ζ_{21}	.2803882
ζ_{22}	1.8023626	.0002229	.2290157	ζ_{22}	.2487423
ζ_{23}	.97855234	.0000684	.0603513	ζ_{23}	.1753809
ζ_{24}	.53137824	.0000077	.0096219	ζ_{24}	.1015503
ζ_{25}	.28857580			ζ_{25}	.0403480
ζ_{26}	.15672251			ζ_{26}	.0122016

Table 63-2. Eu ^{8}S (29s, 22p, 16d, 13f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	29	22	16	13
Nuclear charge	63	Number of closed shells	6	4	2	0
No. of electrons	63	Open-shell occupation	0	0	0	7

Coupling coefficients

$K_0^{ff} = -0.14285714$ $K_2^{ff} = -0.03809524$ $K_4^{ff} = -0.02597403$ $K_6^{ff} = -0.03330003$

Total energy	Potential energy	Kinetic energy	Virial theorem
-10423.54261	-20847.08150	10423.53890	-2.00000035

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1690.69649	-272.31584	-61.31194	-12.74470	-1.81596	-0.17094
ζ_1	80436410.	.0000018	-.0000006	.0000003	-.0000001	.0000000	.0000000
ζ_2	16321621.	.0000100	-.0000033	.0000015	-.0000007	.0000003	-.0000001
ζ_3	3844767.1	.0000565	-.0000186	.0000085	-.0000041	.0000015	-.0000004
ζ_4	1039712.5	.0002606	-.0000857	.0000394	-.0000188	.0000071	-.0000018
ζ_5	318630.03	.0010332	-.0003400	.0001565	-.0000746	.0000283	-.0000072
ζ_6	109098.24	.0035592	-.0011745	.0005406	-.0002577	.0000977	-.0000249
ζ_7	41116.631	.0108440	-.0036040	.0016616	-.0007917	.0003001	-.0000764
ζ_8	16802.347	.0295063	-.0099675	.0046027	-.0021960	.0008326	-.0002122
ζ_9	7338.6820	.0715501	-.0250419	.0116370	-.0055534	.0021055	-.0005364
ζ_{10}	3380.7004	.1510840	-.0568151	.0266519	-.0127661	.0048444	-.0012346
ζ_{11}	1623.5023	.2613886	-.1130678	.0542952	-.0260910	.0099065	-.0025240
ζ_{12}	804.70053	.3260364	-.1814314	.0905528	-.0440373	.0167669	-.0042755
ζ_{13}	408.32055	.2292497	-.1790958	.0965077	-.0475001	.0181276	-.0046196
ζ_{14}	210.73262	.0597856	.0524573	-.0347233	.0173099	-.0066185	.0016815
ζ_{15}	110.06498	.0028957	.4731344	-.3825585	.2091718	-.0816866	.0209080
ζ_{16}	57.959196	.0001405	.5012794	-.5854602	.3454502	-.1373069	.0351710
ζ_{17}	30.687642	-.0000172	.1432903	.0298074	-.0159610	.0055092	-.0013281
ζ_{18}	16.305432	-.0001010	.0074090	.8329289	-.8849777	.4032830	-.1053726
ζ_{19}	8.6826473	.0000655	-.0001578	.4318844	-.5717884	.2635707	-.0686756
ζ_{20}	4.6295690	-.0000474	.0001790	.0405047	.6516095	-.3802292	.1015358
ζ_{21}	2.4703193	.0000416	-.0004449	.0052075	.7727177	-.7111363	.2087435
ζ_{22}	1.3186826	-.0000298	.0003160	-.0012989	.1632548	-.1859615	.0492030
ζ_{23}	.70406925	.0000213	-.0002331	.0008190	.0095177	.5547106	-.1811096
ζ_{24}	.37595085	-.0000152	.0001752	-.0006368	-.0004472	.6534792	-.3091279
ζ_{25}	.20075372	.0000102	-.0001177	.0003716	.0015214	.2021186	-.2585100
ζ_{26}	.10720183	-.0000064	.0000749	-.0002342	-.0008920	.0065754	.0521247
ζ_{27}	.05724565	.0000035	-.0000414	.0001269	.0005234	.0021877	.4584866
ζ_{28}	.03056914	-.0000015	.0000175	-.0000533	-.0002272	-.0008694	.5309484
ζ_{29}	.01632390	.0000004	-.0000041	.0000125	.0000544	.0002006	.2013338

Table 63-2. Eu ^{8}S (29s, 22p, 16d, 13f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-258.36280	-55.07379	-10.24609	-1.06542
ζ_5	318630.03	.0000055	-.0000027	.0000012	-.0000004
ζ_6	109098.24	.0000256	-.0000125	.0000059	-.0000020
ζ_7	41116.631	.0001352	-.0000652	.0000303	-.0000104
ζ_8	16802.347	.0005844	-.0002848	.0001337	-.0000459
ζ_9	7338.6820	.0022705	-.0011016	.0005141	-.0001758
ζ_{10}	3380.7004	.0079261	-.0038993	.0018328	-.0006291
ζ_{11}	1623.5023	.0248367	-.0123202	.0057803	-.0019798
ζ_{12}	804.70053	.0691750	-.0354411	.0168014	-.0057761
ζ_{13}	408.32055	.1622171	-.0864429	.0412083	-.0141597
ζ_{14}	210.73262	.2951525	-.1685615	.0820166	-.0283479
ζ_{15}	110.06498	.3535663	-.2068341	.1006568	-.0346858
ζ_{16}	57.959196	.2135586	-.0273909	-.0015748	.0014590
ζ_{17}	30.687642	.0455049	.3840143	-.2743915	.1024234
ζ_{18}	16.305432	.0021875	.5249093	-.4156326	.1569890
ζ_{19}	8.6826473	-.0001190	.1947779	.0614807	-.0472509
ζ_{20}	4.6295690	.0000049	.0214268	.5673442	-.2851163
ζ_{21}	2.4703193	-.0001188	.0002626	.4545256	-.2744446
ζ_{22}	1.3186826	.0000642	.0009469	.1039348	.0847160
ζ_{23}	.70406925	-.0000446	-.0005969	.0100511	.4147307
ζ_{24}	.37595085	.0000264	.0003519	-.0006955	.4644611
ζ_{25}	.20075372	-.0000120	-.0001663	.0007186	.1937555
ζ_{26}	.10720183	.0000031	.0000460	-.0002578	.0416843

	Orbital	3d	4d		4f
	Energy	-43.60257	-5.77997		-0.71166
ζ_8	16802.347	.0000073	-.0000033		
ζ_9	7338.6820	.0000337	-.0000162		
ζ_{10}	3380.7004	.0001816	-.0000831		
ζ_{11}	1623.5023	.0008664	-.0004103		
ζ_{12}	804.70053	.0036567	-.0017028		
ζ_{13}	408.32055	.0141915	-.0067420	ζ_{13}	.0003037
ζ_{14}	210.73262	.0462964	-.0220179	ζ_{14}	.0009976
ζ_{15}	110.06498	.1263986	-.0617196	ζ_{15}	.0048861
ζ_{16}	57.959196	.2578303	-.1257116	ζ_{16}	.0178539
ζ_{17}	30.687642	.3646502	-.1709725	ζ_{17}	.0515417
ζ_{18}	16.305432	.2922054	-.0651626	ζ_{18}	.1222378
ζ_{19}	8.6826473	.0997107	.2321184	ζ_{19}	.2170944
ζ_{20}	4.6295690	.0129289	.4262133	ζ_{20}	.2786267
ζ_{21}	2.4703193	.0003455	.3477273	ζ_{21}	.2806433
ζ_{22}	1.3186826	.0003152	.1277333	ζ_{22}	.2183599
ζ_{23}	.70406925	-.0000329	.0272574	ζ_{23}	.1398901
ζ_{24}	.37595085			ζ_{24}	.0628120
ζ_{25}	.20075372			ζ_{25}	.0245683

Table 64. Gd ^{7}F (30s, 23p, 17d, 14f; 30 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	30	23	17	14
Nuclear charge	64	Number of closed shells	6	4	2	0
No. of electrons	64	Open-shell occupation	0	0	0	8

Coupling coefficients

$K_0^{ff} = -0.10714286$ $K_2^{ff} = -0.02023810$ $K_4^{ff} = -0.01379870$ $K_6^{ff} = -0.01769064$

Total energy	Potential energy	Kinetic energy	Virial theorem
-10820.61709	-21641.23390	10820.61680	-2.00000003

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1747.06099	-282.33135	-63.76269	-13.22089	-1.85965	-0.17276
ζ_1	99561132.	.0000014	-.0000005	.0000002	-.0000001	.0000000	.0000000
ζ_2	20624281.	.0000076	-.0000025	.0000012	-.0000006	.0000002	-.0000001
ζ_3	4915676.1	.0000430	-.0000142	.0000065	-.0000031	.0000012	-.0000003
ζ_4	1335116.8	.0001981	-.0000652	.0000301	-.0000144	.0000054	-.0000014
ζ_5	408659.11	.0007904	-.0002602	.0001200	-.0000573	.0000216	-.0000055
ζ_6	139242.24	.0027504	-.0009079	.0004191	-.0002003	.0000757	-.0000191
ζ_7	52129.432	.0084861	-.0028168	.0013005	-.0006206	.0002342	-.0000591
ζ_8	21160.470	.0234272	-.0078846	.0036509	-.0017466	.0006602	-.0001666
ζ_9	9192.8532	.0578575	-.0200435	.0093106	-.0044470	.0016783	-.0004234
ζ_{10}	4222.2510	.1256158	-.0462357	.0217055	-.0104235	.0039450	-.0009958
ζ_{11}	2027.6361	.2285416	-.0944687	.0450549	-.0216273	.0081664	-.0020606
ζ_{12}	1008.2627	.3151169	-.1615749	.0800049	-.0389611	.0148043	-.0037388
ζ_{13}	514.90461	.2705583	-.1923411	.1006365	-.0491374	.0185778	-.0046881
ζ_{14}	268.23716	.1037527	-.0532995	.0312794	-.0167399	.0066416	-.0016875
ζ_{15}	141.77901	.0096895	.3307514	-.2454005	.1328245	-.0519140	.0131606
ζ_{16}	75.716402	.0007399	.5521033	-.5612285	.3180528	-.1238419	.0313686
ζ_{17}	40.726744	-.0003754	.2718433	-.3165629	.2161413	-.0907579	.0232288
ζ_{18}	22.012504	.0001989	.0304891	.5957785	-.5414086	.2411063	-.0621942
ζ_{19}	11.935319	-.0001930	.0015980	.7012909	-.9120636	.4189616	-.1082999
ζ_{20}	6.4843798	.0001414	-.0007320	.1391654	.1176201	-.0707495	.0182800
ζ_{21}	3.5272155	-.0000973	.0002412	.0200740	.8621053	-.6038852	.1668213
ζ_{22}	1.9200081	.0000739	-.0002798	-.0074814	.4642296	-.5517110	.1635050
ζ_{23}	1.0455466	-.0000535	.0001912	.0064978	.0333369	.1757726	-.0634894
ζ_{24}	.56947008	.0000381	-.0001268	-.0049688	.0145445	.6532766	-.2232303
ζ_{25}	.31019857	-.0000268	.0000929	.0035002	-.0079112	.5037183	-.3135857
ζ_{26}	.16897651	.0000180	-.0000611	-.0024237	.0060477	.0795722	-.1681009
ζ_{27}	.09204908	-.0000113	.0000382	.0015325	-.0038171	.0111382	.1559063
ζ_{28}	.05014349	.0000061	-.0000208	-.0008417	.0021216	-.0048286	.5053779
ζ_{29}	.02731556	-.0000026	.0000086	.0003518	-.0008936	.0021698	.4681806
ζ_{30}	.01488010	.0000006	-.0000020	-.0000814	.0002078	-.0005246	.1319126

Table 64. Gd ^{7}F (30s, 23p, 17d, 14f; 30 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-268.11289	-57.38027	-10.65032	-1.08831
ζ_5	408659.11	.0000038	-.0000018	.0000009	-.0000003
ζ_6	139242.24	.0000178	-.0000086	.0000040	-.0000014
ζ_7	52129.432	.0000954	-.0000463	.0000218	-.0000075
ζ_8	21160.470	.0004171	-.0002030	.0000948	-.0000323
ζ_9	9192.8532	.0016422	-.0008011	.0003770	-.0001287
ζ_{10}	4222.2510	.0057807	-.0028380	.0013300	-.0004527
ζ_{11}	2027.6361	.0183372	-.0091069	.0042995	-.0014687
ζ_{12}	1008.2627	.0518771	-.0263584	.0124525	-.0042465
ζ_{13}	514.90461	.1264402	-.0667668	.0319474	-.0109409
ζ_{14}	268.23716	.2473432	-.1382530	.0667465	-.0228572
ζ_{15}	141.77901	.3454117	-.2051832	.1013108	-.0349334
ζ_{16}	75.716402	.2758102	-.1237009	.0535319	-.0177822
ζ_{17}	40.726744	.0945237	.2113332	-.1499287	.0548523
ζ_{18}	22.012504	.0088796	.5273122	-.4095031	.1550627
ζ_{19}	11.935319	.0003735	.3460244	-.2065108	.0674868
ζ_{20}	6.4843798	-.0002009	.0645877	.3788821	-.1858553
ζ_{21}	3.5272155	-.0000030	.0065510	.5677991	-.3111319
ζ_{22}	1.9200081	-.0000442	-.0010704	.2633487	-.1322751
ζ_{23}	1.0455466	.0000202	.0011330	.0340265	.2475600
ζ_{24}	.56947008	-.0000122	-.0007477	.0049229	.4539390
ζ_{25}	.31019857	.0000070	.0004299	-.0011576	.3770455
ζ_{26}	.16897651	-.0000030	-.0001948	.0006663	.1136818
ζ_{27}	.09204908	.0000007	.0000517	-.0002274	.0227511

	Orbital	3d	4d		4f
	Energy	-45.64387	-6.04982		-0.69515
ζ_8	21160.470	.0000047	-.0000022		
ζ_9	9192.8532	.0000222	-.0000105		
ζ_{10}	4222.2510	.0001210	-.0000565		
ζ_{11}	2027.6361	.0005773	-.0002720		
ζ_{12}	1008.2627	.0024425	-.0011490		
ζ_{13}	514.90461	.0095434	-.0045295	ζ_{13}	.0001878
ζ_{14}	268.23716	.0319077	-.0152417	ζ_{14}	.0006178
ζ_{15}	141.77901	.0907652	-.0441460	ζ_{15}	.0030230
ζ_{16}	75.716402	.2025172	-.0998218	ζ_{16}	.0114588
ζ_{17}	40.726744	.3276328	-.1584115	ζ_{17}	.0351609
ζ_{18}	22.012504	.3395648	-.1339901	ζ_{18}	.0874020
ζ_{19}	11.935319	.1741609	.0926436	ζ_{19}	.1736713
ζ_{20}	6.4843798	.0363755	.3577310	ζ_{20}	.2498079
ζ_{21}	3.5272155	.0029466	.4055120	ζ_{21}	.2774302
ζ_{22}	1.9200081	.0002565	.2333686	ζ_{22}	.2467218
ζ_{23}	1.0455466	.0000833	.0630141	ζ_{23}	.1757890
ζ_{24}	.56947008	.0000130	.0106151	ζ_{24}	.1050490
ζ_{25}	.31019857			ζ_{25}	.0435957
ζ_{26}	.16897651			ζ_{26}	.0151111

Table 65. Tb ^{6}H (30s, 23p, 17d, 14f; 30 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	30	23	17	14
Nuclear charge	65	Number of closed shells	6	4	2	0
No. of electrons	65	Open-shell occupation	0	0	0	9

Coupling coefficients

$K_0^{ff} = -0.07936508$ $K_2^{ff} = -0.01348227$ $K_4^{ff} = -0.00776403$ $K_6^{ff} = -0.00707610$

Total energy	Potential energy	Kinetic energy	Virial theorem
-11226.56814	-22453.13610	11226.56800	-2.00000001

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1804.34264	-292.51308	-66.24269	-13.69395	-1.90122	-0.17448
ζ_1	104753910.	.0000014	-.0000005	.0000002	-.0000001	.0000000	.0000000
ζ_2	21602526.	.0000075	-.0000025	.0000011	-.0000005	.0000002	-.0000001
ζ_3	5133150.0	.0000424	-.0000140	.0000065	-.0000031	.0000012	-.0000003
ζ_4	1391727.0	.0001958	-.0000645	.0000298	-.0000143	.0000054	-.0000013
ζ_5	425700.10	.0007809	-.0002574	.0001190	-.0000569	.0000214	-.0000053
ζ_6	145077.23	.0027151	-.0008971	.0004151	-.0001987	.0000748	-.0000187
ζ_7	54359.475	.0083647	-.0027790	.0012860	-.0006148	.0002311	-.0000578
ζ_8	22093.452	.0230538	-.0077648	.0036040	-.0017273	.0006502	-.0001626
ζ_9	9612.3772	.0568683	-.0197073	.0091752	-.0043901	.0016500	-.0004126
ζ_{10}	4421.7340	.1234868	-.0454277	.0213742	-.0102828	.0038757	-.0009696
ζ_{11}	2126.5727	.2253152	-.0929050	.0443927	-.0213464	.0080271	-.0020075
ζ_{12}	1058.8756	.3131754	-.1596439	.0791704	-.0386187	.0146129	-.0036575
ζ_{13}	541.37723	.2736125	-.1928402	.1009564	-.0493764	.0185929	-.0046508
ζ_{14}	282.29901	.1084101	-.0613366	.0360058	-.0191323	.0075180	-.0018907
ζ_{15}	149.32689	.0107415	.3177303	-.2349138	.1272743	-.0495343	.0124430
ζ_{16}	79.795601	.0007829	.5537747	-.5587590	.3168772	-.1228622	.0308469
ζ_{17}	42.940829	-.0003958	.2834819	-.3382317	.2296153	-.0956216	.0242296
ζ_{18}	23.217374	.0002210	.0333541	.5767873	-.5223339	.2312356	-.0590704
ζ_{19}	12.591961	-.0002127	.0017481	.7155863	-.9247980	.4230023	-.1083796
ζ_{20}	6.8425242	.0001563	-.0008034	.1481997	.0901548	-.0569750	.0146525
ζ_{21}	3.7226285	-.0001086	.0003110	.0207918	.8581446	-.5913586	.1611573
ζ_{22}	2.0266475	.0000824	-.0003384	-.0074747	.4798529	-.5592392	.1641468
ζ_{23}	1.1037439	-.0000597	.0002349	.0065684	.0373003	.1520227	-.0553652
ζ_{24}	.60123073	.0000426	-.0001592	-.0050213	.0148386	.6407348	-.2142299
ζ_{25}	.32753146	-.0000300	.0001160	.0035420	-.0080309	.5182961	-.3082846
ζ_{26}	.17843556	.0000202	-.0000767	-.0024547	.0061743	.0906916	-.1775036
ζ_{27}	.09721110	-.0000126	.0000481	.0015524	-.0038975	.0111908	.1322730
ζ_{28}	.05296051	.0000069	-.0000262	-.0008528	.0021682	-.0044907	.4908218
ζ_{29}	.02885286	-.0000029	.0000109	.0003565	-.0009136	.0020319	.4785530
ζ_{30}	.01571903	.0000007	-.0000025	-.0000824	.0002125	-.0004930	.1545125

Table 65. Tb ^{6}H (30s, 23p, 17d, 14f; 30 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-278.02926	-59.71555	-11.05115	-1.10948
ζ_5	425700.10	.0000037	-.0000018	.0000009	-.0000003
ζ_6	145077.23	.0000175	-.0000085	.0000040	-.0000013
ζ_7	54359.475	.0000937	-.0000456	.0000215	-.0000073
ζ_8	22093.452	.0004085	-.0001993	.0000933	-.0000316
ζ_9	9612.3772	.0016044	-.0007851	.0003704	-.0001258
ζ_{10}	4421.7340	.0056349	-.0027739	.0013027	-.0004408
ζ_{11}	2126.5727	.0178573	-.0088942	.0042095	-.0014297
ζ_{12}	1058.8756	.0505334	-.0257346	.0121827	-.0041299
ζ_{13}	541.37723	.1235541	-.0653838	.0313597	-.0106776
ζ_{14}	282.29901	.2432952	-.1361928	.0658798	-.0224269
ζ_{15}	149.32689	.3440438	-.2049751	.1014813	-.0347918
ζ_{16}	79.795601	.2805170	-.1300688	.0572445	-.0189777
ζ_{17}	42.940829	.0990802	.2006154	-.1436096	.0522583
ζ_{18}	23.217374	.0096775	.5259115	-.4089046	.1538682
ζ_{19}	12.591961	.0004136	.3547085	-.2178774	.0718704
ζ_{20}	6.8425242	-.0002146	.0680095	.3693920	-.1805739
ζ_{21}	3.7226285	.0000100	.0069707	.5695702	-.3082808
ζ_{22}	2.0266475	-.0000544	-.0011292	.2711640	-.1388566
ζ_{23}	1.1037439	.0000273	.0012081	.0361326	.2361876
ζ_{24}	.60123073	-.0000168	-.0007935	.0052165	.4473392
ζ_{25}	.32753146	.0000096	.0004575	-.0012160	.3848006
ζ_{26}	.17843556	-.0000042	-.0002074	.0007127	.1220917
ζ_{27}	.09721110	.0000010	.0000549	-.0002388	.0250285

	Orbital	3d	4d		4f
	Energy	-47.71323	-6.31592		-0.69536
ζ_8	22093.452	.0000047	-.0000022		
ζ_9	9612.3772	.0000216	-.0000102		
ζ_{10}	4421.7340	.0001180	-.0000554		
ζ_{11}	2126.5727	.0005611	-.0002654		
ζ_{12}	1058.8756	.0023719	-.0011213		
ζ_{13}	541.37723	.0092653	-.0044161	ζ_{13}	.0001855
ζ_{14}	282.29901	.0310728	-.0149130	ζ_{14}	.0006102
ζ_{15}	149.32689	.0887887	-.0433677	ζ_{15}	.0029942
ζ_{16}	79.795601	.1996761	-.0989332	ζ_{16}	.0113909
ζ_{17}	42.940829	.3260373	-.1586099	ζ_{17}	.0351913
ζ_{18}	23.217374	.3416100	-.1366705	ζ_{18}	.0878070
ζ_{19}	12.591961	.1776067	.0885412	ζ_{19}	.1744465
ζ_{20}	6.8425242	.0376310	.3558300	ζ_{20}	.2502217
ζ_{21}	3.7226285	.0031663	.4061964	ζ_{21}	.2764458
ζ_{22}	2.0266475	.0002727	.2362127	ζ_{22}	.2454495
ζ_{23}	1.1037439	.0001036	.0644115	ζ_{23}	.1752850
ζ_{24}	.60123073	.0000155	.0111446	ζ_{24}	.1061466
ζ_{25}	.32753146			ζ_{25}	.0448871
ζ_{26}	.17843556			ζ_{26}	.0166026

Table 66. Dy ^{5}I (29s, 22p, 16d, 13f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	29	22	16	13
Nuclear charge	66	Number of closed shells	6	4	2	0
No. of electrons	66	Open-shell occupation	0	0	0	10

Coupling coefficients

$K_0^{ff} = -0.05714286$ $K_2^{ff} = -0.01079365$ $K_4^{ff} = -0.00465958$ $K_6^{ff} = -0.00053482$

Total energy	Potential energy	Kinetic energy	Virial theorem
-11641.45209	-23282.90450	11641.45240	-1.99999997

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1862.54414	-302.86411	-68.75552	-14.16663	-1.94134	-0.17612
ζ_1	89049143.	.0000018	-.0000006	.0000003	-.0000001	.0000000	.0000000
ζ_2	17865654.	.0000101	-.0000033	.0000015	-.0000007	.0000003	-.0000001
ζ_3	4178570.2	.0000574	-.0000189	.0000088	-.0000042	.0000016	-.0000004
ζ_4	1125969.3	.0002655	-.0000875	.0000406	-.0000194	.0000073	-.0000018
ζ_5	344820.74	.0010514	-.0003470	.0001609	-.0000771	.0000289	-.0000072
ζ_6	118226.68	.0036094	-.0011947	.0005538	-.0002654	.0000994	-.0000246
ζ_7	44675.255	.0109462	-.0036494	.0016949	-.0008122	.0003042	-.0000754
ζ_8	18315.837	.0296424	-.0100461	.0046718	-.0022409	.0008392	-.0002082
ζ_9	8025.7757	.0715858	-.0251393	.0117704	-.0056497	.0021166	-.0005249
ζ_{10}	3707.7406	.1507624	-.0568898	.0268774	-.0129425	.0048509	-.0012033
ζ_{11}	1784.4165	.2606518	-.1131268	.0547588	-.0264767	.0099357	-.0024643
ζ_{12}	885.66895	.3256993	-.1817566	.0913815	-.0446748	.0167966	-.0041688
ζ_{13}	449.65438	.2298868	-.1800780	.0980073	-.0486243	.0183587	-.0045550
ζ_{14}	232.01828	.0601399	.0527101	-.0356708	.0181186	-.0069025	.0017095
ζ_{15}	121.07907	.0028515	.4771068	-.3904894	.2149265	-.0828459	.0206344
ζ_{16}	63.670778	.0001506	.5021254	-.5964388	.3572226	-.1407584	.0351065
ζ_{17}	33.651083	-.0000316	.1393635	.0573671	-.0404689	.0163898	-.0040569
ζ_{18}	17.842343	-.0000870	.0066126	.8503902	-.9268428	.4173414	-.1060322
ζ_{19}	9.4789696	.0000572	-.0002236	.4066400	-.5177384	.2352116	-.0595985
ζ_{20}	5.0416778	-.0000406	.0002224	.0367421	.7004655	-.4105317	.1069095
ζ_{21}	2.6833194	.0000361	-.0004580	.0033012	.7417423	-.6904555	.1967593
ζ_{22}	1.4286300	-.0000258	.0003333	-.0000783	.1414463	-.1409266	.0350587
ζ_{23}	0.7607488	.0000183	-.0002453	-.0001088	.0097858	.5597900	-.1768336
ζ_{24}	.40513184	-.0000130	.0001831	.0000451	-.0015765	.6357511	-.2963353
ζ_{25}	.21575706	.0000087	-.0001233	-.0000907	.0021905	.1920399	-.2456298
ζ_{26}	.11490486	-.0000055	.0000785	.0000601	-.0013280	.0069798	.0471695
ζ_{27}	.06119461	.0000030	-.0000434	-.0000358	.0007649	.0015619	.4483804
ζ_{28}	.03259029	-.0000013	.0000184	.0000157	-.0003306	-.0005945	.5249910
ζ_{29}	.01735654	.0000003	-.0000044	-.0000038	.0000791	.0001340	.2136392

Table 66. Dy ^{5}I (29s, 22p, 16d, 13f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-288.11492	-62.08317	-11.45121	-1.12946
ζ_5	344820.74	.0000057	-.0000028	.0000013	-.0000004
ζ_6	118226.68	.0000262	-.0000129	.0000061	-.0000021
ζ_7	44675.255	.0001379	-.0000671	.0000314	-.0000105
ζ_8	18315.837	.0005924	-.0002913	.0001378	-.0000465
ζ_9	8025.7757	.0022888	-.0011204	.0005261	-.0001768
ζ_{10}	3707.7406	.0079570	-.0039515	.0018718	-.0006318
ζ_{11}	1784.4165	.0248816	-.0124567	.0058829	-.0019799
ζ_{12}	885.66895	.0692866	-.0358463	.0171278	-.0057900
ζ_{13}	449.65438	.1627181	-.0875859	.0420513	-.0141998
ζ_{14}	232.01828	.2965730	-.1712797	.0840716	-.0285783
ζ_{15}	121.07907	.3546502	-.2093991	.1025789	-.0347252
ζ_{16}	63.670778	.2119172	-.0220322	-.0051612	.0026902
ζ_{17}	33.651083	.0434952	.4016882	-.2929764	.1078205
ζ_{18}	17.842343	.0019572	.5221291	-.4147707	.1534252
ζ_{19}	9.4789696	-.0001668	.1800812	.1011292	-.0635252
ζ_{20}	5.0416778	.0000413	.0190616	.5819238	-.2896109
ζ_{21}	2.6833194	-.0001338	-.0002577	.4311402	-.2540087
ζ_{22}	1.4286300	.0000783	.0012309	.0904298	.1059810
ζ_{23}	0.7607488	-.0000531	-.0007852	.0090319	.4151686
ζ_{24}	.40513184	.0000312	.0004667	-.0009450	.4537576
ζ_{25}	.21575706	-.0000142	-.0002186	.0008016	.1889026
ζ_{26}	.11490486	.0000037	.0000598	-.0002714	.0404809

	Orbital	3d	4d		4f
	Energy	-49.81408	-6.58062		-0.70309
ζ_8	18315.837	.0000076	-.0000035		
ζ_9	8025.7757	.0000347	-.0000170		
ζ_{10}	3707.7406	.0001871	-.0000866		
ζ_{11}	1784.4165	.0008870	-.0004263		
ζ_{12}	885.66895	.0037473	-.0017687		
ζ_{13}	449.65438	.0145411	-.0070099	ζ_{13}	.0003375
ζ_{14}	232.01828	.0476296	-.0229872	ζ_{14}	.0011089
ζ_{15}	121.07907	.1302629	-.0646045	ζ_{15}	.0054811
ζ_{16}	63.670778	.2652875	-.1313267	ζ_{16}	.0199883
ζ_{17}	33.651083	.3698134	-.1749560	ζ_{17}	.0578634
ζ_{18}	17.842343	.2837132	-.0504258	ζ_{18}	.1350931
ζ_{19}	9.4789696	.0900277	.2579141	ζ_{19}	.2301037
ζ_{20}	5.0416778	.0109558	.4324942	ζ_{20}	.2821292
ζ_{21}	2.6833194	.0003115	.3299498	ζ_{21}	.2726450
ζ_{22}	1.4286300	.0003585	.1131152	ζ_{22}	.2065243
ζ_{23}	0.7607488	-.0000199	.0228208	ζ_{23}	.1321825
ζ_{24}	.40513184			ζ_{24}	.0600066
ζ_{25}	.21575706			ζ_{25}	.0253974

Table 67. Ho ^{4}I (29s, 22p, 16d, 13f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	29	22	16	13
Nuclear charge	67	Number of closed shells	6	4	2	0
No. of electrons	67	Open-shell occupation	0	0	0	11

Coupling coefficients

$K_0^{ff} = -0.03896104$ $K_2^{ff} = -0.00671652$ $K_4^{ff} = -0.00234827$ $K_6^{ff} = 0.00148445$

Total energy	Potential energy	Kinetic energy	Virial theorem
-12065.28927	-24130.57800	12065.28880	-2.00000003

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1921.67137	-313.39084	-71.30823	-14.64429	-1.98147	-0.17774
ζ_1	92107305.	.0000018	-.0000006	.0000003	-.0000001	.0000000	.0000000
ζ_2	18510170.	.0000100	-.0000033	.0000015	-.0000007	.0000003	-.0000001
ζ_3	4332794.1	.0000570	-.0000188	.0000087	-.0000042	.0000016	-.0000004
ζ_4	1167647.0	.0002635	-.0000870	.0000404	-.0000194	.0000072	-.0000018
ζ_5	357439.12	.0010444	-.0003450	.0001603	-.0000769	.0000287	-.0000071
ζ_6	122465.24	.0035897	-.0011893	.0005525	-.0002651	.0000989	-.0000243
ζ_7	46238.049	.0108998	-.0036372	.0016929	-.0008124	.0003029	-.0000745
ζ_8	18941.345	.0295482	-.0100229	.0046712	-.0022438	.0008367	-.0002059
ζ_9	8294.5473	.0714161	-.0251002	.0117778	-.0056616	.0021119	-.0005195
ζ_{10}	3830.3772	.1504877	-.0568283	.0269075	-.0129753	.0048424	-.0011915
ζ_{11}	1843.2198	.2603012	-.1130368	.0548385	-.0265559	.0099227	-.0024410
ζ_{12}	915.00959	.3255676	-.1817131	.0915679	-.0448308	.0167837	-.0041321
ζ_{13}	464.75386	.2303900	-.1804868	.0984679	-.0489414	.0183990	-.0045274
ζ_{14}	239.97083	.0606488	.0511659	-.0348306	.0177422	-.0067290	.0016514
ζ_{15}	125.33782	.0029022	.4754203	-.3899987	.2150321	-.0825417	.0203944
ζ_{16}	65.977677	.0001565	.5034427	-.5992315	.3598990	-.1412164	.0349266
ζ_{17}	34.910053	-.0000359	.1408850	.0542533	-.0391667	.0158280	-.0038716
ζ_{18}	18.532533	-.0000834	.0066723	.8507751	-.9290646	.4164559	-.1049427
ζ_{19}	9.8582777	.0000548	-.0001797	.4087725	-.5192003	.2345974	-.0588750
ζ_{20}	5.2503585	-.0000391	.0001971	.0375298	.6951631	-.4049372	.1043664
ζ_{21}	2.7981490	.0000351	-.0004377	.0032210	.7431577	-.6839254	.1929880
ζ_{22}	1.4917950	-.0000252	.0003192	.0000124	.1455995	-.1501485	.0375992
ζ_{23}	0.7954723	.0000180	-.0002356	-.0001635	.0097626	.5439840	-.1692220
ζ_{24}	.42420547	-.0000128	.0001762	.0000877	-.0013352	.6384658	-.2899791
ζ_{25}	.22622566	.0000086	-.0001186	-.0001209	.0020503	.2045184	-.2459330
ζ_{26}	.12064588	-.0000054	.0000755	.0000795	-.0012322	.0081039	.0256192
ζ_{27}	.06434052	.0000030	-.0000418	-.0000469	.0007122	.0018821	.4342902
ζ_{28}	.03431287	-.0000013	.0000177	.0000205	-.0003079	-.0007392	.5213249
ζ_{29}	.01829909	.0000003	-.0000042	-.0000049	.0000736	.0001697	.2431144

Table 67. Ho ^{4}I (29s, 22p, 16d, 13f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-298.37617	-64.49017	-11.85569	-1.14931
ζ_5	357439.12	.0000056	-.0000027	.0000013	-.0000004
ζ_6	122465.24	.0000261	-.0000128	.0000061	-.0000020
ζ_7	46238.049	.0001373	-.0000669	.0000314	-.0000105
ζ_8	18941.345	.0005903	-.0002911	.0001380	-.0000463
ζ_9	8294.5473	.0022834	-.0011209	.0005273	-.0001762
ζ_{10}	3830.3772	.0079423	-.0039550	.0018770	-.0006297
ζ_{11}	1843.2198	.0248407	-.0124719	.0059012	-.0019743
ζ_{12}	915.00959	.0691591	-.0358818	.0171781	-.0057717
ζ_{13}	464.75386	.1624020	-.0876787	.0421803	-.0141591
ζ_{14}	239.97083	.2960591	-.1715105	.0843648	-.0285040
ζ_{15}	125.33782	.3544961	-.2100397	.1031253	-.0347089
ζ_{16}	65.977677	.2125182	-.0229822	-.0047419	.0025496
ζ_{17}	34.910053	.0438379	.4016774	-.2943136	.1076648
ζ_{18}	18.532533	.0019702	.5222622	-.4154852	.1527765
ζ_{19}	9.8582777	-.0001615	.1804406	.1014270	-.0633647
ζ_{20}	5.2503585	.0000411	.0192542	.5800214	-.2864789
ζ_{21}	2.7981490	-.0001323	-.0002558	.4316279	-.2522817
ζ_{22}	1.4917950	.0000777	.0012526	.0920792	.1003905
ζ_{23}	0.7954723	-.0000527	-.0007927	.0091802	.4067269
ζ_{24}	.42420547	.0000311	.0004722	-.0008780	.4548146
ζ_{25}	.22622566	-.0000141	-.0002209	.0007884	.1964782
ζ_{26}	.12064588	.0000037	.0000603	-.0002652	.0440745

	Orbital	3d	4d		4f
	Energy	-51.95333	-6.84866		-0.70840
ζ_8	18941.345	.0000076	-.0000035		
ζ_9	8294.5473	.0000348	-.0000170		
ζ_{10}	3830.3772	.0001880	-.0000874		
ζ_{11}	1843.2198	.0008905	-.0004294		
ζ_{12}	915.00959	.0037628	-.0017835		
ζ_{13}	464.75386	.0145861	-.0070583	ζ_{13}	.0003468
ζ_{14}	239.97083	.0477645	-.0231492	ζ_{14}	.0011350
ζ_{15}	125.33782	.1305426	-.0650099	ζ_{15}	.0056164
ζ_{16}	65.977677	.2657767	-.1321619	ζ_{16}	.0204263
ζ_{17}	34.910053	.3699121	-.1755866	ζ_{17}	.0591165
ζ_{18}	18.532533	.2826932	-.0489909	ζ_{18}	.1373053
ζ_{19}	9.8582777	.0894049	.2597331	ζ_{19}	.2318412
ζ_{20}	5.2503585	.0109317	.4315736	ζ_{20}	.2817169
ζ_{21}	2.7981490	.0003499	.3286329	ζ_{21}	.2704980
ζ_{22}	1.4917950	.0003692	.1128987	ζ_{22}	.2043254
ζ_{23}	0.7954723	-.0000122	.0231435	ζ_{23}	.1315420
ζ_{24}	.42420547			ζ_{24}	.0601281
ζ_{25}	.22622566			ζ_{25}	.0266292

Table 68. Er ^{3}H (29s, 22p, 16d, 13f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	29	22	16	13
Nuclear charge	68	Number of closed shells	6	4	2	0
No. of electrons	68	Open-shell occupation	0	0	0	12

Coupling coefficients

$K_0^{ff} = -0.02380952$ $K_2^{ff} = -0.00202822$ $K_4^{ff} = -0.00057939$ $K_6^{ff} = 0.00087595$

Total energy	Potential energy	Kinetic energy	Virial theorem
-12498.15221	-24996.30500	12498.15280	-1.99999995

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-1981.72438	-324.09338	-73.90107	-15.12710	-2.02164	-0.17935
ζ_1	94399000.	.0000018	-.0000006	.0000003	-.0000001	.0000000	.0000000
ζ_2	19023385.	.0000100	-.0000033	.0000015	-.0000007	.0000003	-.0000001
ζ_3	4462014.1	.0000570	-.0000188	.0000088	-.0000042	.0000016	-.0000004
ζ_4	1204085.5	.0002630	-.0000869	.0000404	-.0000194	.0000072	-.0000018
ζ_5	368852.85	.0010418	-.0003445	.0001604	-.0000771	.0000286	-.0000070
ζ_6	126393.56	.0035818	-.0011878	.0005529	-.0002657	.0000986	-.0000241
ζ_7	47705.397	.0108858	-.0036359	.0016960	-.0008150	.0003027	-.0000739
ζ_8	19528.605	.0295499	-.0100326	.0046851	-.0022531	.0008366	-.0002042
ζ_9	8543.2389	.0715319	-.0251661	.0118350	-.0056976	.0021168	-.0005166
ζ_{10}	3940.5275	.1509519	-.0570707	.0270780	-.0130719	.0048573	-.0011857
ζ_{11}	1893.7238	.2612823	-.1136752	.0552881	-.0268196	.0099819	-.0024364
ζ_{12}	938.76927	.3263274	-.1826960	.0922883	-.0452300	.0168569	-.0041171
ζ_{13}	476.13878	.2294778	-.1803880	.0988188	-.0492585	.0184575	-.0045070
ζ_{14}	245.49396	.0593978	.0560187	-.0382990	.0197126	-.0074814	.0018244
ζ_{15}	128.03749	.0027564	.4822020	-.3987431	.2202743	-.0841524	.0206243
ζ_{16}	67.302120	.0001262	.4999573	-.6012284	.3636377	-.1423931	.0349516
ζ_{17}	35.560188	-.0000167	.1347943	.0817416	-.0621384	.0256926	-.0063021
ζ_{18}	18.851030	-.0000967	.0061082	.8588507	-.9504547	.4244240	-.1060619
ζ_{19}	10.013646	.0000663	-.0003238	.3884426	-.4781552	.2145962	-.0534301
ζ_{20}	5.3256696	-.0000474	.0002966	.0350751	.7237542	-.4241190	.1086817
ζ_{21}	2.8343429	.0000409	-.0005005	.0018956	.7224743	-.6743785	.1888473
ζ_{22}	1.5089971	-.0000295	.0003684	.0008706	.1312214	-.1206461	.0288741
ζ_{23}	0.8035315	.0000210	-.0002705	-.0008166	.0101367	.5548261	-.1714933
ζ_{24}	.42791071	-.0000149	.0002003	.0005616	-.0021985	.6277833	-.2878210
ζ_{25}	.22788619	.0000100	-.0001349	-.0004430	.0025751	.1921812	-.2391784
ζ_{26}	.12136347	-.0000063	.0000857	.0002847	-.0015758	.0078264	.0349214
ζ_{27}	.06463377	.0000034	-.0000474	-.0001606	.0009027	.0013116	.4373162
ζ_{28}	.03442162	-.0000014	.0000201	.0000688	-.0003894	-.0004850	.5195065
ζ_{29}	.01833171	.0000003	-.0000048	-.0000164	.0000931	.0001074	.2340343

Table 68. Er ^{3}H (29s, 22p, 16d, 13f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-308.81313	-66.93677	-12.26474	-1.16905
ζ_5	368852.85	.0000056	-.0000027	.0000013	-.0000004
ζ_6	126393.56	.0000260	-.0000129	.0000061	-.0000020
ζ_7	47705.397	.0001372	-.0000671	.0000315	-.0000104
ζ_8	19528.605	.0005911	-.0002923	.0001388	-.0000463
ζ_9	8543.2389	.0022909	-.0011276	.0005312	-.0001764
ζ_{10}	3940.5275	.0079879	-.0039886	.0018968	-.0006328
ζ_{11}	1893.7238	.0250406	-.0126081	.0059744	-.0019867
ζ_{12}	938.76927	.0698512	-.0363530	.0174410	-.0058268
ζ_{13}	476.13878	.1641313	-.0889263	.0428550	-.0142993
ζ_{14}	245.49396	.2986653	-.1737392	.0856857	-.0287894
ζ_{15}	128.03749	.3548817	-.2105698	.1034628	-.0345998
ζ_{16}	67.302120	.2091002	-.0157447	-.0092115	.0040748
ζ_{17}	35.560188	.0415665	.4143423	-.3058736	.1114005
ζ_{18}	18.851030	.0018055	.5177012	-.4107849	.1497303
ζ_{19}	10.013646	-.0002003	.1701845	.1265384	-.0735688
ζ_{20}	5.3256696	.0000677	.0178406	.5868754	-.2895547
ζ_{21}	2.8343429	-.0001454	-.0005912	.4171734	-.2414962
ζ_{22}	1.5089971	.0000882	.0014259	.0840339	.1144356
ζ_{23}	0.8035315	-.0000591	-.0009123	.0086610	.4111161
ζ_{24}	.42791071	.0000347	.0005432	-.0010647	.4486879
ζ_{25}	.22788619	-.0000158	-.0002534	.0008473	.1897482
ζ_{26}	.12136347	.0000041	.0000689	-.0002789	.0416326

	Orbital	3d	4d		4f
	Energy	-54.13118	-7.12014		-0.71152
ζ_8	19528.605	.0000077	-.0000036		
ζ_9	8543.2389	.0000351	-.0000173		
ζ_{10}	3940.5275	.0001908	-.0000890		
ζ_{11}	1893.7238	.0009047	-.0004379		
ζ_{12}	938.76927	.0038400	-.0018267		
ζ_{13}	476.13878	.0149079	-.0072417	ζ_{13}	.0003635
ζ_{14}	245.49396	.0489281	-.0238098	ζ_{14}	.0011944
ζ_{15}	128.03749	.1335782	-.0668104	ζ_{15}	.0059304
ζ_{16}	67.302120	.2707606	-.1351487	ζ_{16}	.0215186
ζ_{17}	35.560188	.3722376	-.1765313	ζ_{17}	.0621780
ζ_{18}	18.851030	.2767762	-.0394320	ζ_{18}	.1430873
ζ_{19}	10.013646	.0839234	.2729723	ζ_{19}	.2371572
ζ_{20}	5.3256696	.0099272	.4335259	ζ_{20}	.2831308
ζ_{21}	2.8343429	.0003027	.3190377	ζ_{21}	.2674838
ζ_{22}	1.5089971	.0003814	.1057052	ζ_{22}	.1995902
ζ_{23}	0.8035315	-.0000131	.0209767	ζ_{23}	.1274601
ζ_{24}	.42791071			ζ_{24}	.0580047
ζ_{25}	.22788619			ζ_{25}	.0255511

Table 69. Tm ^{2}F (29s, 22p, 16d, 13f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	29	22	16	13
Nuclear charge	69	Number of closed shells	6	4	2	0
No. of electrons	69	Open-shell occupation	0	0	0	13

Coupling coefficients

$K_0^{ff} = -0.01098901$ $K_2^{ff} = 0.00022542$ $K_4^{ff} = 0.00015369$ $K_6^{ff} = 0.00019704$

Total energy	Potential energy	Kinetic energy	Virial theorem
-12940.17380	-25880.34830	12940.17450	-1.99999995

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2042.69846	-334.96660	-76.52860	-15.61098	-2.06077	-0.18091
ζ_1	101177770.	.0000017	-.0000006	.0000003	-.0000001	.0000000	.0000000
ζ_2	20223019.	.0000097	-.0000032	.0000015	-.0000007	.0000003	-.0000001
ζ_3	4720909.3	.0000552	-.0000182	.0000085	-.0000041	.0000015	-.0000004
ζ_4	1271557.9	.0002549	-.0000843	.0000393	-.0000189	.0000070	-.0000017
ζ_5	389652.93	.0010080	-.0003336	.0001557	-.0000749	.0000277	-.0000067
ζ_6	133768.92	.0034539	-.0011463	.0005346	-.0002572	.0000951	-.0000230
ζ_7	50625.499	.0104582	-.0034949	.0016334	-.0007857	.0002905	-.0000704
ζ_8	20785.060	.0283137	-.0096136	.0044981	-.0021659	.0008008	-.0001940
ζ_9	9117.6234	.0685227	-.0240749	.0113409	-.0054642	.0020209	-.0004895
ζ_{10}	4214.5378	.1452243	-.0546958	.0259864	-.0125614	.0046481	-.0011262
ζ_{11}	2028.2635	.2543330	-.1096302	.0533443	-.0258867	.0095897	-.0023230
ζ_{12}	1006.0628	.3255793	-.1792361	.0904765	-.0443939	.0164779	-.0039947
ζ_{13}	510.16951	.2394646	-.1853926	.1012036	-.0503779	.0187729	-.0045487
ζ_{14}	262.80143	.0669790	.0339071	-.0239672	.0121284	-.0045587	.0010996
ζ_{15}	136.85775	.0033424	.4645741	-.3787192	.2090926	-.0795539	.0193530
ζ_{16}	71.795533	.0002745	.5168674	-.6130407	.3687469	-.1433780	.0349131
ζ_{17}	37.845084	-.0001219	.1496694	.0338073	-.0254865	.0102300	-.0024451
ζ_{18}	20.009699	-.0000176	.0068954	.8582387	-.9386495	.4165675	-.1032832
ζ_{19}	10.599279	.0000054	-.0000404	.4145437	-.5218141	.2336661	-.0577147
ζ_{20}	5.6206007	-.0000025	.0001147	.0367687	.7064504	-.4088066	.1036691
ζ_{21}	2.9822990	.0000081	-.0003740	.0034573	.7374076	-.6738339	.1865974
ζ_{22}	1.5829137	-.0000057	.0002765	-.0001973	.1413194	-.1404613	.0348039
ζ_{23}	0.8402926	.0000040	-.0002055	-.0000127	.0090064	.5436723	-.1661272
ζ_{24}	.44610181	-.0000030	.0001549	-.0000118	-.0011165	.6323912	-.2827528
ζ_{25}	.23683695	.0000019	-.0001044	-.0000505	.0018493	.2025513	-.2414781
ζ_{26}	.12573873	-.0000012	.0000667	.0000350	-.0011062	.0076008	.0249463
ζ_{27}	.06675592	.0000007	-.0000370	-.0000221	.0006409	.0019886	.4299976
ζ_{28}	.03544140	-.0000003	.0000157	.0000099	-.0002779	-.0007908	.5205292
ζ_{29}	.01881620	.0000001	-.0000037	-.0000024	.0000667	.0001832	.2445657

Table 69. Tm ^{2}F (29s, 22p, 16d, 13f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-319.42073	-69.41756	-12.67439	-1.18790
ζ_5	389652.93	.0000054	-.0000026	.0000012	-.0000004
ζ_6	133768.92	.0000248	-.0000123	.0000058	-.0000019
ζ_7	50625.499	.0001300	-.0000637	.0000300	-.0000099
ζ_8	20785.060	.0005570	-.0002762	.0001314	-.0000436
ζ_9	9117.6234	.0021518	-.0010613	.0005008	-.0001653
ζ_{10}	4214.5378	.0074923	-.0037496	.0017853	-.0005919
ζ_{11}	2028.2635	.0235387	-.0118690	.0056329	-.0018619
ζ_{12}	1006.0628	.0660661	-.0344101	.0165238	-.0054857
ζ_{13}	510.16951	.1572091	-.0851475	.0410846	-.0136258
ζ_{14}	262.80143	.2918012	-.1695696	.0836529	-.0279244
ζ_{15}	136.85775	.3579524	-.2140105	.1056152	-.0351386
ζ_{16}	71.795533	.2204411	-.0332704	.0010111	.0005544
ζ_{17}	37.845084	.0464244	.3997258	-.2949804	.1066354
ζ_{18}	20.009699	.0020623	.5286209	-.4215858	.1530972
ζ_{19}	10.599279	-.0001679	.1814407	.1064306	-.0648369
ζ_{20}	5.6206007	.0000555	.0188922	.5855836	-.2858345
ζ_{21}	2.9822990	-.0001397	-.0002586	.4268125	-.2450667
ζ_{22}	1.5829137	.0000846	.0012517	.0886186	.1049384
ζ_{23}	0.8402926	-.0000571	-.0007890	.0086493	.4059705
ζ_{24}	.44610181	.0000336	.0004729	-.0008590	.4515568
ζ_{25}	.23683695	-.0000153	-.0002215	.0007668	.1965133
ζ_{26}	.12573873	.0000040	.0000606	-.0002554	.0435891

	Orbital	3d	4d		4f
	Energy	-56.34225	-7.39135		-0.71903
ζ_8	20785.060	.0000072	-.0000033		
ζ_9	9117.6234	.0000327	-.0000162		
ζ_{10}	4214.5378	.0001761	-.0000823		
ζ_{11}	2028.2635	.0008383	-.0004074		
ζ_{12}	1006.0628	.0035584	-.0016969		
ζ_{13}	510.16951	.0139401	-.0067933	ζ_{13}	.0003377
ζ_{14}	262.80143	.0462615	-.0225681	ζ_{14}	.0011298
ζ_{15}	136.85775	.1283944	-.0643879	ζ_{15}	.0056386
ζ_{16}	71.795533	.2655483	-.1331371	ζ_{16}	.0208537
ζ_{17}	37.845084	.3731987	-.1786094	ζ_{17}	.0611615
ζ_{18}	20.009699	.2845509	-.0478515	ζ_{18}	.1423445
ζ_{19}	10.599279	.0883568	.2672587	ζ_{19}	.2377625
ζ_{20}	5.6206007	.0105777	.4350485	ζ_{20}	.2842428
ζ_{21}	2.9822990	.0003764	.3236821	ζ_{21}	.2681584
ζ_{22}	1.5829137	.0003908	.1081754	ζ_{22}	.1999590
ζ_{23}	0.8402926	-.0000051	.0215032	ζ_{23}	.1277942
ζ_{24}	.44610181			ζ_{24}	.0584666
ζ_{25}	.23683695			ζ_{25}	.0261732

Table 70. Yb ^{1}S (29s, 22p, 16d, 13f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	29	22	16	13
Nuclear charge	70	Number of closed shells	6	4	2	1
No. of electrons	70	Open-shell occupation	0	0	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-13391.45555	-26782.91230	13391.45680	-1.99999990

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2104.59204	-346.00883	-79.18919	-16.09478	-2.09862	-0.18241
ζ_1	100674930.	.0000017	-.0000006	.0000003	-.0000001	.0000000	.0000000
ζ_2	20366645.	.0000099	-.0000033	.0000015	-.0000007	.0000003	-.0000001
ζ_3	4788484.0	.0000560	-.0000185	.0000087	-.0000042	.0000015	-.0000004
ζ_4	1293624.2	.0002584	-.0000855	.0000399	-.0000192	.0000071	-.0000017
ζ_5	396317.20	.0010245	-.0003394	.0001587	-.0000764	.0000281	-.0000068
ζ_6	135714.08	.0035278	-.0011719	.0005476	-.0002637	.0000970	-.0000233
ζ_7	51164.021	.0107442	-.0035946	.0016833	-.0008107	.0002984	-.0000718
ζ_8	20915.018	.0292355	-.0099410	.0046604	-.0022457	.0008264	-.0001988
ζ_9	9136.5004	.0709510	-.0249941	.0118007	-.0056937	.0020966	-.0005043
ζ_{10}	4208.5020	.1501303	-.0568148	.0270605	-.0130893	.0048204	-.0011597
ζ_{11}	2020.1938	.2606310	-.1134420	.0553973	-.0269362	.0099371	-.0023903
ζ_{12}	1000.5685	.3267072	-.1828722	.0927407	-.0455405	.0168205	-.0040489
ζ_{13}	507.16114	.2308606	-.1815429	.0999135	-.0499623	.0185605	-.0044659
ζ_{14}	261.38690	.0601308	.0544581	-.0376441	.0195212	-.0073562	.0017666
ζ_{15}	136.30236	.0027878	.4824859	-.4013106	.2222755	-.0841524	.0203269
ζ_{16}	71.646406	.0001312	.5014431	-.6071082	.3695059	-.1435313	.0347120
ζ_{17}	37.860708	-.0000212	.1344547	.0897227	-.0709834	.0293566	-.0070942
ζ_{18}	20.075352	-.0000923	.0059399	.8636182	-.9630518	.4260494	-.1048910
ζ_{19}	10.667319	.0000642	-.0003397	.3816998	-.4597173	.2037468	-.0498738
ζ_{20}	5.6753615	-.0000459	.0003183	.0347779	.7305301	-.4250390	.1070999
ζ_{21}	3.0216325	.0000397	-.0005094	.0011993	.7140037	-.6601829	.1818234
ζ_{22}	1.6093698	-.0000287	.0003776	.0013617	.1292523	-.1184901	.0280396
ζ_{23}	0.8573401	.0000205	-.0002777	-.0011721	.0101866	.5402094	-.1629987
ζ_{24}	.45676054	-.0000146	.0002053	.0008224	-.0022941	.6257827	-.2791104
ζ_{25}	.24335468	.0000098	-.0001384	-.0006205	.0026356	.2017801	-.2353299
ζ_{26}	.12965713	-.0000062	.0000880	.0003974	-.0016123	.0091048	.0128127
ζ_{27}	.06908039	.0000034	-.0000486	-.0002231	.0009237	.0014539	.4228907
ζ_{28}	.03680556	-.0000014	.0000206	.0000953	-.0003984	-.0005515	.5106080
ζ_{29}	.01960975	.0000003	-.0000049	-.0000226	.0000952	.0001242	.2674526

Table 70. Yb ^{1}S (29s, 22p, 16d, 13f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-330.19733	-71.93089	-13.08347	-1.20567
ζ_5	396317.20	.0000055	-.0000027	.0000013	-.0000004
ζ_6	135714.08	.0000255	-.0000127	.0000061	-.0000020
ζ_7	51164.021	.0001350	-.0000663	.0000312	-.0000102
ζ_8	20915.018	.0005833	-.0002898	.0001381	-.0000455
ζ_9	9136.5004	.0022671	-.0011215	.0005297	-.0001737
ζ_{10}	4208.5020	.0079262	-.0039772	.0018971	-.0006250
ζ_{11}	2020.1938	.0249101	-.0126065	.0059902	-.0019673
ζ_{12}	1000.5685	.0696404	-.0364272	.0175304	-.0057840
ζ_{13}	507.16114	.1639859	-.0893357	.0431819	-.0142308
ζ_{14}	261.38690	.2989060	-.1748902	.0865561	-.0287221
ζ_{15}	136.30236	.3553991	-.2121087	.1045466	-.0345340
ζ_{16}	71.646406	.2090334	-.0143434	-.0103862	.0044538
ζ_{17}	37.860708	.0411130	.4203349	-.3130622	.1126585
ζ_{18}	20.075352	.0017573	.5160469	-.4091558	.1470596
ζ_{19}	10.667319	-.0002160	.1658570	.1391821	-.0779973
ζ_{20}	5.6753615	.0000846	.0173841	.5875406	-.2861809
ζ_{21}	3.0216325	-.0001528	-.0007368	.4107170	-.2337070
ζ_{22}	1.6093698	.0000947	.0015257	.0821193	.1137189
ζ_{23}	0.8573401	-.0000631	-.0009723	.0085448	.4024953
ζ_{24}	.45676054	.0000370	.0005801	-.0010686	.4470314
ζ_{25}	.24335468	-.0000168	-.0002700	.0008551	.1962121
ζ_{26}	.12965713	.0000044	.0000732	-.0002768	.0451412

	Orbital	3d	4d		4f
	Energy	-58.58489	-7.66114		-0.73215
ζ_8	20915.018	.0000077	-.0000036		
ζ_9	9136.5004	.0000350	-.0000173		
ζ_{10}	4208.5020	.0001912	-.0000899		
ζ_{11}	2020.1938	.0009079	-.0004420		
ζ_{12}	1000.5685	.0038678	-.0018521		
ζ_{13}	507.16114	.0150341	-.0073486	ζ_{13}	.0003812
ζ_{14}	261.38690	.0494770	-.0242428	ζ_{14}	.0012546
ζ_{15}	136.30236	.1351582	-.0680651	ζ_{15}	.0062519
ζ_{16}	71.646406	.2737847	-.1376539	ζ_{16}	.0226418
ζ_{17}	37.860708	.3736931	-.1777563	ζ_{17}	.0654288
ζ_{18}	20.075352	.2728036	-.0326896	ζ_{18}	.1489399
ζ_{19}	10.667319	.0806138	.2816909	ζ_{19}	.2420633
ζ_{20}	5.6753615	.0094462	.4330150	ζ_{20}	.2834608
ζ_{21}	3.0216325	.0003309	.3126637	ζ_{21}	.2635184
ζ_{22}	1.6093698	.0003991	.1020486	ζ_{22}	.1945700
ζ_{23}	0.8573401	-.0000047	.0202923	ζ_{23}	.1240691
ζ_{24}	.45676054			ζ_{24}	.0565556
ζ_{25}	.24335468			ζ_{25}	.0257621

Table 71. Lu ^{2}D (28s, 21p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	21	18	12
Nuclear charge	71	Number of closed shells	6	4	2	1
No. of electrons	71	Open-shell occupation	0	0	1	0

Coupling coefficients

$K_0^{dd} = -1.80000000$ $K_2^{dd} = 0.05714286$ $K_4^{dd} = 0.05714286$

Total energy	Potential energy	Kinetic energy	Virial theorem
-13851.80635	-27703.61320	13851.80690	-1.99999996

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2167.73075	-357.57173	-82.26815	-16.93731	-2.31670	-0.19878
ζ_1	57801052.	.0000036	-.0000012	.0000006	-.0000003	.0000001	.0000000
ζ_2	11862288.	.0000199	-.0000066	.0000031	-.0000015	.0000006	-.0000001
ζ_3	2811063.3	.0001126	-.0000373	.0000174	-.0000084	.0000032	-.0000008
ζ_4	760961.32	.0005196	-.0001722	.0000806	-.0000389	.0000147	-.0000037
ζ_5	232413.98	.0020737	-.0006882	.0003221	-.0001555	.0000585	-.0000148
ζ_6	79005.098	.0072023	-.0024027	.0011266	-.0005444	.0002049	-.0000520
ζ_7	29466.468	.0220572	-.0074501	.0034953	-.0016879	.0006346	-.0001609
ζ_8	11886.092	.0594715	-.0206991	.0097711	-.0047299	.0017812	-.0004518
ζ_9	5114.2865	.1381924	-.0512874	.0243995	-.0118181	.0044444	-.0011270
ζ_{10}	2317.5570	.2600018	-.1102609	.0537105	-.0262033	.0098893	-.0025093
ζ_{11}	1093.6304	.3461802	-.1886730	.0954317	-.0468602	.0176581	-.0044784
ζ_{12}	532.25428	.2488948	-.1946080	.1070756	-.0539386	.0205596	-.0052249
ζ_{13}	265.04840	.0601199	.0672590	-.0465090	.0249033	-.0097881	.0025014
ζ_{14}	134.19447	.0023030	.5265876	-.4495609	.2496795	-.0962906	.0244857
ζ_{15}	68.741037	-.0001006	.4848568	-.6081960	.3813149	-.1533236	.0392460
ζ_{16}	35.495090	.0001658	.0975510	.2699840	-.2277174	.0994190	-.0257702
ζ_{17}	18.425667	-.0002386	.0045076	.8814381	-.0518262	.4776606	-.1239177
ζ_{18}	9.5974190	.0001851	-.0019030	.2545937	-.1675773	.0712951	-.0189237
ζ_{19}	5.0095204	-.0001352	.0014136	.0252186	.8917498	-.5858931	.1606967
ζ_{20}	2.6180297	.0001036	-.0012540	-.0067846	.5489605	-.6202078	.1836567
ζ_{21}	1.3691561	-.0000750	.0009290	.0064478	.0421507	.1611520	-.0557397
ζ_{22}	0.7162894	.0000532	-.0006650	-.0049851	.0131451	.7091885	-.2567327
ζ_{23}	0.3748004	-.0000372	.0004721	.0035298	-.0070054	.4744050	-.3241490
ζ_{24}	.19613027	.0000250	-.0003181	-.0024418	.0052704	.0555390	-.1135800
ζ_{25}	.10263651	-.0000157	.0002009	.0015543	-.0033329	.0086700	.2574061
ζ_{26}	.05371098	.0000087	-.0001115	-.0008676	.0018741	-.0040860	.5512893
ζ_{27}	.02810770	-.0000037	.0000478	.0003733	-.0008103	.0019038	.3875087
ζ_{28}	.01470915	.0000009	-.0000115	-.0000900	.0001960	-.0004752	.0562720

Table 71. Lu ^{2}D (28s, 21p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-341.48957	-74.85973	-13.84450	-1.37554
ζ_5	232413.98	.0000148	-.0000073	.0000035	-.0000012
ζ_6	79005.098	.0000697	-.0000343	.0000162	-.0000055
ζ_7	29466.468	.0003768	-.0001873	.0000897	-.0000305
ζ_8	11886.092	.0016521	-.0008190	.0003878	-.0001310
ζ_9	5114.2865	.0065175	-.0032680	.0015652	-.0005324
ζ_{10}	2317.5570	.0225151	-.0113997	.0054308	-.0018384
ζ_{11}	1093.6304	.0680734	-.0355569	.0171756	-.0058494
ζ_{12}	532.25428	.1694541	-.0924857	.0448395	-.0152337
ζ_{13}	265.04840	.3170152	-.1861744	.0926452	-.0317514
ζ_{14}	134.19447	.3669084	-.2179631	.1072955	-.0364643
ζ_{15}	68.741037	.1929732	.0304841	-.0385715	.0145433
ζ_{16}	35.495090	.0288626	.4931755	-.3766305	.1409876
ζ_{17}	18.425667	.0012392	.4788422	-.3602609	.1300267
ζ_{18}	9.5974190	-.0005191	.1087262	.2963457	-.1493912
ζ_{19}	5.0095204	.0002813	.0113660	.6165129	-.3276906
ζ_{20}	2.6180297	-.0002642	-.0025846	.3079350	-.1629540
ζ_{21}	1.3691561	.0001755	.0023920	.0346379	.2602229
ζ_{22}	0.7162894	-.0001132	-.0015921	.0059181	.4883498
ζ_{23}	0.3748004	.0000657	.0009365	-.0020624	.3638136
ζ_{24}	.19613027	-.0000301	-.0004366	.0010814	.0917948
ζ_{25}	.10263651	.0000081	.0001186	-.0003313	.0150718

	Orbital	3d	4d	5d		4f
	Energy	-61.23582	-8.26436	-0.24322		-1.07641
ζ_9	5114.2865	.0001916	-.0000917	.0000184		
ζ_{10}	2317.5570	.0007128	-.0003485	.0000705		
ζ_{11}	1093.6304	.0037330	-.0018020	.0003613		
ζ_{12}	532.25428	.0152899	-.0075194	.0015191	ζ_{12}	.0003854
ζ_{13}	265.04840	.0537895	-.0265752	.0053537	ζ_{13}	.0014733
ζ_{14}	134.19447	.1505280	-.0764328	.0155003	ζ_{14}	.0075522
ζ_{15}	68.741037	.3030481	-.1532863	.0309844	ζ_{15}	.0282106
ζ_{16}	35.495090	.3869882	-.1790086	.0358026	ζ_{16}	.0818360
ζ_{17}	18.425667	.2409961	.0255596	-.0114229	ζ_{17}	.1808317
ζ_{18}	9.5974190	.0542872	.3542657	-.0850896	ζ_{18}	.2730778
ζ_{19}	5.0095204	.0054458	.4398642	-.1039000	ζ_{19}	.2996263
ζ_{20}	2.6180297	-.0002763	.2516953	-.0322905	ζ_{20}	.2520342
ζ_{21}	1.3691561	.0006802	.0607137	.1060690	ζ_{21}	.1694402
ζ_{22}	0.7162894	-.0003784	.0079837	.2352392	ζ_{22}	.0806005
ζ_{23}	0.3748004	.0002668	-.0002318	.2992603	ζ_{23}	.0364543
ζ_{24}	.19613027	-.0001564	.0005816	.3095046		
ζ_{25}	.10263651	.0000751	-.0002643	.1915136		
ζ_{26}	.05371098	-.0000222	.0000894	.1204870		

Table 72. Hf ^{3}F (28s, 21p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	21	18	12
Nuclear charge	72	Number of closed shells	6	4	2	1
No. of electrons	72	Open-shell occupation	0	0	2	0

Coupling coefficients

$K_0^{dd} = -0.80000000$ $K_2^{dd} = -0.10612245$ $K_4^{dd} = 0.03673469$

Total energy	Potential energy	Kinetic energy	Virial theorem
-14321.24839	-28642.49630	14321.24790	-2.00000003

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2231.81039	-369.32922	-85.41135	-17.79712	-2.51907	-0.20892
ζ_1	68974306.	.0000030	-.0000010	.0000005	-.0000002	.0000001	.0000000
ζ_2	13971077.	.0000170	-.0000056	.0000026	-.0000013	.0000005	-.0000001
ζ_3	3282919.8	.0000964	-.0000320	.0000150	-.0000073	.0000028	-.0000007
ζ_4	884868.43	.0004467	-.0001481	.0000695	-.0000336	.0000129	-.0000033
ζ_5	270041.82	.0017804	-.0005913	.0002772	-.0001343	.0000515	-.0000133
ζ_6	91980.342	.0061607	-.0020546	.0009648	-.0004673	.0001793	-.0000464
ζ_7	34445.907	.0187954	-.0063400	.0029792	-.0014446	.0005542	-.0001433
ζ_8	13970.465	.0506670	-.0175341	.0082820	-.0040164	.0015410	-.0003986
ζ_9	6048.4376	.1189635	-.0435665	.0207239	-.0100812	.0038697	-.0010011
ζ_{10}	2758.5728	.2313009	-.0949778	.0460916	-.0224849	.0086388	-.0022351
ζ_{11}	1310.0120	.3335612	-.1708411	.0857092	-.0422572	.0162662	-.0042096
ζ_{12}	641.40463	.2837555	-.2056799	.1108239	-.0553211	.0213701	-.0055330
ζ_{13}	321.18484	.0954853	-.0271627	.0142844	-.0077158	.0030020	-.0007781
ζ_{14}	163.44732	.0056607	.4256573	-.3357421	.1854963	-.0731486	.0189923
ζ_{15}	84.116482	.0006573	.5589343	-.6453524	.3876322	-.1561924	.0406728
ζ_{16}	43.620388	-.0003937	.1790281	-.0413856	.0286899	-.0120847	.0031561
ζ_{17}	22.733522	.0001858	.0081883	.8710729	-.9486416	.4366265	-.1157227
ζ_{18}	11.885517	-.0001467	.0002131	.4404570	-.5612218	.2643645	-.0704166
ζ_{19}	6.2259588	.0001089	-.0000184	.0356394	.7375290	-.4488345	.1232136
ζ_{20}	3.2649834	-.0000726	-.0002928	.0046683	.7384250	-.7353379	.2206341
ζ_{21}	1.7132613	.0000521	.0002300	-.0012393	.1218593	-.0782154	.0192230
ζ_{22}	0.8992993	-.0000370	-.0001723	.0006608	.0083540	.6738995	-.2406564
ζ_{23}	0.4721178	.0000255	.0001321	-.0004885	-.0018926	.5844319	-.3347203
ζ_{24}	.24787032	-.0000171	-.0000895	.0002771	.0021838	.1224397	-.1772069
ζ_{25}	.13013947	.0000107	.0000573	-.0001704	-.0013508	.0047234	.1724361
ζ_{26}	.06832769	-.0000059	-.0000319	.0000919	.0007751	.0001452	.4984523
ζ_{27}	.03587444	.0000025	.0000137	-.0000389	-.0003367	.0000922	.4645455
ζ_{28}	.01883535	-.0000006	-.0000033	.0000093	.0000815	-.0000309	.1218266

Table 72. Hf ^{3}F (28s, 21p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-352.97546	-77.85189	-14.62140	-1.53205
ζ_5	270041.82	.0000120	-.0000060	.0000029	-.0000010
ζ_6	91980.342	.0000560	-.0000276	.0000131	-.0000046
ζ_7	34445.907	.0003003	-.0001497	.0000718	-.0000251
ζ_8	13970.465	.0013066	-.0006481	.0003087	-.0001072
ζ_9	6048.4376	.0051155	-.0025692	.0012330	-.0004303
ζ_{10}	2758.5728	.0176871	-.0089386	.0042792	-.0014884
ζ_{11}	1310.0120	.0540157	-.0280968	.0135871	-.0047478
ζ_{12}	641.40463	.1392331	-.0752004	.0365637	-.0127597
ζ_{13}	321.18484	.2791478	-.1615393	.0801805	-.0281705
ζ_{14}	163.44732	.3716916	-.2254852	.1127903	-.0395374
ζ_{15}	84.116482	.2483543	-.0683651	.0213074	-.0067580
ζ_{16}	43.620388	.0558940	.3840316	-.2869889	.1095705
ζ_{17}	22.733522	.0024950	.5495671	-.4432158	.1697990
ζ_{18}	11.885517	-.0002042	.1906998	.1022971	-.0672208
ζ_{19}	6.2259588	.0001003	.0187459	.6064956	-.3177437
ζ_{20}	3.2649834	-.0001736	-.0002743	.4216232	-.2579319
ζ_{21}	1.7132613	.0001125	.0011820	.0755004	.1601179
ζ_{22}	0.8992993	-.0000746	-.0007837	.0071431	.4785611
ζ_{23}	0.4721178	.0000443	.0004631	-.0012715	.4227020
ζ_{24}	.24787032	-.0000202	-.0002210	.0008515	.1351706
ζ_{25}	.13013947	.0000054	.0000601	-.0002704	.0237008

	Orbital	3d	4d	5d		4f
	Energy	-63.94828	-8.88049	-0.32425		-1.42977
ζ_9	6048.4376	.0001407	-.0000676	.0000152		
ζ_{10}	2758.5728	.0005205	-.0002575	.0000587		
ζ_{11}	1310.0120	.0026928	-.0013037	.0002932		
ζ_{12}	641.40463	.0112121	-.0055568	.0012627	ζ_{12}	.0002651
ζ_{13}	321.18484	.0403307	-.0199706	.0045165	ζ_{13}	.0010519
ζ_{14}	163.44732	.1191643	-.0607309	.0138420	ζ_{14}	.0053634
ζ_{15}	84.116482	.2610224	-.1334200	.0303202	ζ_{15}	.0213876
ζ_{16}	43.620388	.3816589	-.1874693	.0425523	ζ_{16}	.0653183
ζ_{17}	22.733522	.2964934	-.0546152	.0076811	ζ_{17}	.1559799
ζ_{18}	11.885517	.0903740	.2779290	-.0771932	ζ_{18}	.2589503
ζ_{19}	6.2259588	.0104802	.4506915	-.1209091	ζ_{19}	.3046762
ζ_{20}	3.2649834	.0000889	.3159575	-.0682536	ζ_{20}	.2701448
ζ_{21}	1.7132613	.0006679	.0950401	.0813514	ζ_{21}	.1857946
ζ_{22}	0.8992993	-.0003352	.0133420	.2393406	ζ_{22}	.0875045
ζ_{23}	0.4721178	.0002442	.0001840	.3205646	ζ_{23}	.0381889
ζ_{24}	.24787032	-.0001439	.0005947	.3176535		
ζ_{25}	.13013947	.0000688	-.0002472	.1866324		
ζ_{26}	.06832769	-.0000204	.0000870	.0997221		

Table 73. Ta ^{4}F (28s, 21p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	21	18	12
Nuclear charge	73	Number of closed shells	6	4	2	1
No. of electrons	73	Open-shell occupation	0	0	3	0

Coupling coefficients

$K_0^{dd} = -0.46666667$ $K_2^{dd} = -0.07891156$ $K_4^{dd} = -0.01541950$

Total energy	Potential energy	Kinetic energy	Virial theorem
-14799.81137	-29599.62210	14799.81080	-2.00000003

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2296.84166	-381.29193	-88.62837	-18.68402	-2.72014	-0.21742
ζ_1	76966188.	.0000027	-.0000009	.0000004	-.0000002	.0000001	.0000000
ζ_2	15476141.	.0000155	-.0000051	.0000024	-.0000012	.0000005	-.0000001
ζ_3	3620868.6	.0000885	-.0000294	.0000138	-.0000067	.0000026	-.0000007
ζ_4	974244.51	.0004102	-.0001361	.0000639	-.0000311	.0000121	-.0000032
ζ_5	297412.10	.0016323	-.0005425	.0002548	-.0001239	.0000484	-.0000126
ζ_6	101491.21	.0056315	-.0018785	.0008834	-.0004292	.0001676	-.0000437
ζ_7	38116.288	.0171318	-.0057768	.0027194	-.0013236	.0005171	-.0001350
ζ_8	15511.147	.0461593	-.0159331	.0075328	-.0036631	.0014302	-.0003734
ζ_9	6738.7622	.1089527	-.0396396	.0188744	-.0092168	.0036038	-.0009412
ζ_{10}	3083.4588	.2155167	-.0870834	.0422022	-.0206269	.0080609	-.0021047
ζ_{11}	1468.5036	.3236363	-.1605517	.0803144	-.0397346	.0155860	-.0040725
ζ_{12}	720.71830	.2995516	-.2072826	.1105541	-.0551153	.0216188	-.0056471
ζ_{13}	361.57748	.1182411	-.0698114	.0402610	-.0214108	.0085874	-.0022532
ζ_{14}	184.25968	.0095252	.3625730	-.2760133	.1524628	-.0613752	.0160996
ζ_{15}	94.920596	.0009499	.5824675	-.6381471	.3774200	-.1537206	.0403621
ζ_{16}	49.254892	-.0006104	.2319051	-.1910444	.1381007	-.0603057	.0160158
ζ_{17}	25.679931	.0003684	.0135404	.8179376	-.8524514	.3983919	-.1067204
ζ_{18}	13.428556	-.0002969	.0014539	.5440817	-.7324022	.3520991	-.0945814
ζ_{19}	7.0346660	.0002206	-.0009289	.0502305	.6192731	-.3704092	.1018221
ζ_{20}	3.6889759	-.0001540	.0003689	.0107152	.8193490	-.7826050	.2366351
ζ_{21}	1.9355845	.0001112	-.0002665	-.0053177	.1747093	-.1877244	.0544791
ζ_{22}	1.0158805	-.0000790	.0001839	.0037545	.0057605	.6634137	-.2409081
ζ_{23}	0.5332504	.0000546	-.0001165	-.0027282	.0015648	.6200638	-.3396563
ζ_{24}	.27992660	-.0000367	.0000783	.0018067	.0000358	.1508237	-.1897605
ζ_{25}	.14694881	.0000231	-.0000484	-.0011456	.0000340	.0030869	.1463413
ζ_{26}	.07714196	-.0000127	.0000266	.0006356	.0000052	.0023000	.4752594
ζ_{27}	.04049634	.0000054	-.0000113	-.0002724	-.0000051	-.0008492	.4767392
ζ_{28}	.02125891	-.0000013	.0000027	.0000654	.0000016	.0002025	.1549178

Table 73. Ta ^{4}F (28s, 21p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-364.66569	-80.91703	-15.42415	-1.68816
ζ_5	297412.10	.0000106	-.0000053	.0000025	-.0000009
ζ_6	101491.21	.0000495	-.0000245	.0000117	-.0000042
ζ_7	38116.288	.0002635	-.0001316	.0000632	-.0000226
ζ_8	15511.147	.0011418	-.0005675	.0002720	-.0000969
ζ_9	6738.7622	.0044506	-.0022379	.0010767	-.0003845
ζ_{10}	3083.4588	.0154087	-.0077923	.0037504	-.0013371
ζ_{11}	1468.5036	.0473312	-.0245810	.0119129	-.0042595
ζ_{12}	720.71830	.1243517	-.0669069	.0326688	-.0116820
ζ_{13}	361.57748	.2583017	-.1483731	.0736760	-.0264760
ζ_{14}	184.25968	.3683896	-.2242134	.1130083	-.0406513
ζ_{15}	94.920596	.2763234	-.1108249	.0464377	-.0161289
ζ_{16}	49.254892	.0749715	.3197522	-.2388126	.0931075
ζ_{17}	25.679931	.0039905	.5693622	-.4637589	.1834257
ζ_{18}	13.428556	.0000565	.2408878	.0036137	-.0249155
ζ_{19}	7.0346660	-.0000686	.0254423	.5834822	-.3096780
ζ_{20}	3.6889759	-.0000679	.0014800	.4744689	-.3012044
ζ_{21}	1.9355845	.0000374	.0001927	.1014413	.1173857
ζ_{22}	1.0158805	-.0000266	-.0001088	.0077022	.4804155
ζ_{23}	0.5332504	.0000171	.0000591	-.0004796	.4408346
ζ_{24}	.27992660	-.0000077	-.0000360	.0005590	.1491394
ζ_{25}	.14694881	.0000021	.0000099	-.0001848	.0263390

	Orbital	3d	4d	5d		4f
	Energy	-66.73205	-9.52009	-0.38762		-1.80432
ζ_9	6738.7622	.0001182	-.0000572	.0000139		
ζ_{10}	3083.4588	.0004353	-.0002169	.0000534		
ζ_{11}	1468.5036	.0022466	-.0010954	.0002663		
ζ_{12}	720.71830	.0094310	-.0047043	.0011551	ζ_{12}	.0002186
ζ_{13}	361.57748	.0344386	-.0171577	.0041938	ζ_{13}	.0008882
ζ_{14}	184.25968	.1046604	-.0535855	.0131960	ζ_{14}	.0045328
ζ_{15}	94.920596	.2396882	-.1236168	.0303827	ζ_{15}	.0186886
ζ_{16}	49.254892	.3738212	-.1878193	.0461762	ζ_{16}	.0589577
ζ_{17}	25.679931	.3214294	-.0887002	.0176966	ζ_{17}	.1460891
ζ_{18}	13.428556	.1126489	.2373079	-.0729808	ζ_{18}	.2541696
ζ_{19}	7.0346660	.0142908	.4504931	-.1315448	ζ_{19}	.3090810
ζ_{20}	3.6889759	.0005079	.3449894	-.0874853	ζ_{20}	.2793926
ζ_{21}	1.9355845	.0005311	.1125576	.0737892	ζ_{21}	.1896607
ζ_{22}	1.0158805	-.0002235	.0158338	.2517148	ζ_{22}	.0861814
ζ_{23}	0.5332504	.0001694	.0005175	.3376988	ζ_{23}	.0335743
ζ_{24}	.27992660	-.0001008	.0004860	.3152842		
ζ_{25}	.14694881	.0000476	-.0001837	.1759157		
ζ_{26}	.07714196	-.0000143	.0000671	.0808693		

Table 74. W ^{5}D (28s, 21p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	21	18	12
Nuclear charge	74	Number of closed shells	6	4	2	1
No. of electrons	74	Open-shell occupation	0	0	4	0

Coupling coefficients

$K_0^{dd} = -0.30000000$ $K_2^{dd} = -0.05000000$ $K_4^{dd} = -0.05000000$

Total energy	Potential energy	Kinetic energy	Virial theorem
-15287.54525	-30575.09660	15287.55130	-1.99999961

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2362.82318	-393.45821	-91.91700	-19.59588	-2.92097	-0.22473
ζ_1	81884798.	.0000026	-.0000009	.0000004	-.0000002	.0000001	.0000000
ζ_2	16569649.	.0000147	-.0000049	.0000023	-.0000011	.0000004	-.0000001
ζ_3	3890365.2	.0000836	-.0000277	.0000131	-.0000064	.0000025	-.0000007
ζ_4	1048059.9	.0003874	-.0001286	.0000605	-.0000295	.0000117	-.0000031
ζ_5	319811.19	.0015441	-.0005135	.0002417	-.0001179	.0000468	-.0000123
ζ_6	108975.64	.0053433	-.0017833	.0008398	-.0004094	.0001625	-.0000425
ζ_7	40849.450	.0163136	-.0055014	.0025943	-.0012673	.0005034	-.0001318
ζ_8	16593.078	.0441368	-.0152225	.0072054	-.0035156	.0013949	-.0003652
ζ_9	7199.0655	.1047261	-.0380018	.0181212	-.0088806	.0035307	-.0009247
ζ_{10}	3292.0533	.2089210	-.0838822	.0406586	-.0199334	.0079153	-.0020721
ζ_{11}	1568.2454	.3188444	-.1561228	.0781043	-.0387705	.0154665	-.0040531
ζ_{12}	770.55433	.3052335	-.2069968	.1100083	-.0549602	.0218902	-.0057316
ζ_{13}	387.34918	.1288394	-.0867392	.0504354	-.0267611	.0109303	-.0028790
ζ_{14}	197.93167	.0120261	.3300985	-.2480322	.1372636	-.0562902	.0148201
ζ_{15}	102.30450	.0010243	.5865669	-.6258948	.3686892	-.1521787	.0400420
ζ_{16}	53.289630	-.0006521	.2609910	-.2643204	.1889115	-.0837452	.0223350
ζ_{17}	27.900012	.0004145	.0184615	.7690110	-.7837108	.3722365	-.1001504
ζ_{18}	14.654497	-.0003410	.0019453	.6031687	-.8204236	.4008986	-.1079348
ζ_{19}	7.7124859	.0002546	-.0012941	.0662186	.5207900	-.3098445	.0847477
ζ_{20}	4.0636568	-.0001794	.0006481	.0134575	.8660079	-.8106612	.2460177
ζ_{21}	2.1424714	.0001303	-.0004872	-.0069567	.2193751	-.2705525	.0808009
ζ_{22}	1.1299396	-.0000928	.0003452	.0050786	.0052823	.6453735	-.2363644
ζ_{23}	0.5960230	.0000644	-.0002300	-.0037195	.0039160	.6467367	-.3409720
ζ_{24}	.31441253	-.0000433	.0001558	.0024894	-.0013684	.1785724	-.1980274
ζ_{25}	.16586220	.0000272	-.0000974	-.0015838	.0009530	.0031837	.1097238
ζ_{26}	.08749804	-.0000150	.0000538	.0008792	-.0005032	.0038367	.4493101
ζ_{27}	.04615832	.0000064	-.0000229	-.0003760	.0002134	-.0015061	.4773898
ζ_{28}	.02435016	-.0000015	.0000055	.0000899	-.0000508	.0003646	.2080525

Table 74. W ^{5}D (28s, 21p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-376.55867	-84.05297	-16.25076	-1.84485
ζ_5	319811.19	.0000098	-.0000049	.0000024	-.0000009
ζ_6	108975.64	.0000460	-.0000228	.0000110	-.0000040
ζ_7	40849.450	.0002457	-.0001229	.0000592	-.0000216
ζ_8	16593.078	.0010691	-.0005327	.0002567	-.0000935
ζ_9	7199.0655	.0041776	-.0021033	.0010153	-.0003701
ζ_{10}	3292.0533	.0145067	-.0073497	.0035552	-.0012958
ζ_{11}	1568.2454	.0446785	-.0232101	.0112864	-.0041204
ζ_{12}	770.55433	.1181183	-.0635496	.0311714	-.0113944
ζ_{13}	387.34918	.2483863	-.1423639	.0708841	-.0260061
ζ_{14}	197.93167	.3640497	-.2219344	.1124848	-.0413894
ζ_{15}	102.30450	.2880771	-.1288240	.0572428	-.0204871
ζ_{16}	53.289630	.0860751	.2827817	-.2126463	.0846255
ζ_{17}	27.900012	.0052926	.5715025	-.4672239	.1895778
ζ_{18}	14.654497	.0002015	.2718794	-.0557390	.0013855
ζ_{19}	7.7124859	-.0001632	.0318720	.5572224	-.3011136
ζ_{20}	4.0636568	-.0000067	.0025106	.5076111	-.3309582
ζ_{21}	2.1424714	-.0000076	-.0003157	.1229644	.0843098
ζ_{22}	1.1299396	.0000026	.0002496	.0087818	.4772770
ζ_{23}	0.5960230	.0000007	-.0001619	.0001064	.4537934
ζ_{24}	.31441253	-.0000001	.0000641	.0003684	.1622812
ζ_{25}	.16586220	.0000001	-.0000177	-.0001238	.0299045

	Orbital	3d	4d	5d		4f
	Energy	-69.58504	-10.18155	-0.44619		-2.19927
ζ_9	7199.0655	.0001093	-.0000534	.0000138		
ζ_{10}	3292.0533	.0004035	-.0002022	.0000528		
ζ_{11}	1568.2454	.0020830	-.0010244	.0002646		
ζ_{12}	770.55433	.0087493	-.0043928	.0011448	ζ_{12}	.0002054
ζ_{13}	387.34918	.0320659	-.0160964	.0041785	ζ_{13}	.0008358
ζ_{14}	197.93167	.0981527	-.0505599	.0132171	ζ_{14}	.0042555
ζ_{15}	102.30450	.2284888	-.1188419	.0310306	ζ_{15}	.0176592
ζ_{16}	53.289630	.3664195	-.1866176	.0487512	ζ_{16}	.0563086
ζ_{17}	27.900012	.3319628	-.1054351	.0236785	ζ_{17}	.1412985
ζ_{18}	14.654497	.1265395	.2109172	-.0703234	ζ_{18}	.2511127
ζ_{19}	7.7124859	.0174326	.4454081	-.1390659	ζ_{19}	.3109065
ζ_{20}	4.0636568	.0008270	.3623663	-.1017375	ζ_{20}	.2838624
ζ_{21}	2.1424714	.0004456	.1254328	.0675105	ζ_{21}	.1902590
ζ_{22}	1.1299396	-.0001525	.0180435	.2601729	ζ_{22}	.0834601
ζ_{23}	0.5960230	.0001206	.0007852	.3464784	ζ_{23}	.0301622
ζ_{24}	.31441253	-.0000728	.0004028	.3126930		
ζ_{25}	.16586220	.0000336	-.0001448	.1677480		
ζ_{26}	.08749804	-.0000103	.0000502	.0732362		

Table 75. Re ^{6}S (28s, 21p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	21	18	12
Nuclear charge	75	Number of closed shells	6	4	2	1
No. of electrons	75	Open-shell occupation	0	0	5	0

Coupling coefficients

$K_0^{dd} = -0.20000000$ $K_2^{dd} = -0.05714286$ $K_4^{dd} = -0.05714286$

Total energy	Potential energy	Kinetic energy	Virial theorem
-15784.53216	-31569.06840	15784.53630	-1.99999973

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2429.75094	-405.82381	-95.27263	-20.52799	-3.11954	-0.23060
ζ_1	86861663.	.0000025	-.0000008	.0000004	-.0000002	.0000001	.0000000
ζ_2	17601376.	.0000141	-.0000047	.0000022	-.0000011	.0000004	-.0000001
ζ_3	4135852.3	.0000801	-.0000266	.0000125	-.0000061	.0000025	-.0000006
ζ_4	1114542.1	.0003709	-.0001232	.0000581	-.0000284	.0000114	-.0000030
ζ_5	340096.12	.0014792	-.0004922	.0002320	-.0001137	.0000458	-.0000119
ζ_6	115868.53	.0051216	-.0017102	.0008066	-.0003946	.0001589	-.0000414
ζ_7	43425.453	.0156505	-.0052789	.0024935	-.0012224	.0004929	-.0001286
ζ_8	17638.220	.0424115	-.0146192	.0069285	-.0033922	.0013659	-.0003562
ζ_9	7653.5125	.1009576	-.0365556	.0174560	-.0085853	.0034650	-.0009041
ζ_{10}	3501.2239	.2028110	-.0809812	.0392682	-.0193145	.0077817	-.0020291
ζ_{11}	1669.0019	.3140802	-.1520167	.0760558	-.0378793	.0153416	-.0040057
ζ_{12}	820.83423	.3099878	-.2063859	.1093795	-.0547875	.0221311	-.0057711
ζ_{13}	413.11758	.1387456	-.1009065	.0587870	-.0311536	.0129167	-.0033911
ζ_{14}	211.39739	.0146299	.3019790	-.2244885	.1244854	-.0519073	.0136262
ζ_{15}	109.43843	.0010834	.5883688	-.6142977	.3611209	-.1509626	.0395521
ζ_{16}	57.104373	-.0006744	.2860194	-.3203787	.2268404	-.1018365	.0270766
ζ_{17}	29.952163	.0004458	.0233768	.7259734	-.7285160	.3512849	-.0942968
ζ_{18}	15.762483	-.0003728	.0023177	.6475771	-.8817019	.4373558	-.1173014
ζ_{19}	8.3119034	.0002792	-.0015704	.0808016	.4457960	-.2650136	.0716568
ζ_{20}	4.3882382	-.0001979	.0008683	.0153704	.8972105	-.8363266	.2534278
ζ_{21}	2.3182716	.0001442	-.0006635	-.0080171	.2512839	-.3232675	.0967074
ζ_{22}	1.2251404	-.0001029	.0004751	.0059494	.0053728	.6431259	-.2366504
ζ_{23}	0.6475567	.0000714	-.0003217	-.0043815	.0054706	.6589714	-.3398344
ζ_{24}	.34229458	-.0000481	.0002183	.0029477	-.0022815	.1927277	-.1964553
ζ_{25}	.18093959	.0000302	-.0001369	-.0018789	.0015524	.0028556	.0871991
ζ_{26}	.09564686	-.0000166	.0000756	.0010435	-.0008342	.0048695	.4349993
ζ_{27}	.05056018	.0000071	-.0000322	-.0004460	.0003552	-.0019631	.4671908
ζ_{28}	.02672678	-.0000017	.0000077	.0001064	-.0000847	.0004776	.2464592

Table 75. Re ^{6}S (28s, 21p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-388.65019	-87.25513	-17.09668	-2.00034
ζ_5	340096.12	.0000093	-.0000046	.0000022	-.0000008
ζ_6	115868.53	.0000434	-.0000216	.0000105	-.0000039
ζ_7	43425.453	.0002317	-.0001161	.0000561	-.0000208
ζ_8	17638.220	.0010093	-.0005041	.0002442	-.0000907
ζ_9	7653.5125	.0039448	-.0019888	.0009636	-.0003579
ζ_{10}	3501.2239	.0137195	-.0069631	.0033847	-.0012581
ζ_{11}	1669.0019	.0423521	-.0220118	.0107429	-.0039959
ζ_{12}	820.83423	.1126810	-.0606287	.0298723	-.0111347
ζ_{13}	413.11758	.2398374	-.1372278	.0685401	-.0256187
ζ_{14}	211.39739	.3601860	-.2197952	.1119659	-.0420283
ζ_{15}	109.43843	.2979676	-.1429667	.0658251	-.0241370
ζ_{16}	57.104373	.0959176	.2533934	-.1924482	.0780702
ζ_{17}	29.952163	.0066020	.5714680	-.4684231	.1942699
ζ_{18}	15.762483	.0003167	.2962326	-.0991085	.0213540
ζ_{19}	8.3119034	-.0002385	.0375710	.5373881	-.2962019
ζ_{20}	4.3882382	.0000441	.0033093	.5305988	-.3540871
ζ_{21}	2.3182716	-.0000451	-.0007006	.1377931	.0661604
ζ_{22}	1.2251404	.0000273	.0005172	.0095850	.4808786
ζ_{23}	0.6475567	-.0000131	-.0003304	.0005095	.4592145
ζ_{24}	.34229458	.0000064	.0001398	.0002457	.1672256
ζ_{25}	.18093959	-.0000016	-.0000385	-.0000814	.0307280

	Orbital	3d	4d	5d		4f
	Energy	-72.50275	-10.86068	-0.51417		-2.61082
ζ_9	7653.5125	.0001020	-.0000502	.0000136		
ζ_{10}	3501.2239	.0003762	-.0001897	.0000520		
ζ_{11}	1669.0019	.0019434	-.0009636	.0002617		
ζ_{12}	820.83423	.0081720	-.0041308	.0011309	ζ_{12}	.0001941
ζ_{13}	413.11758	.0301035	-.0152257	.0041550	ζ_{13}	.0007931
ζ_{14}	211.39739	.0929139	-.0481660	.0132299	ζ_{14}	.0040425
ζ_{15}	109.43843	.2197259	-.1152290	.0316368	ζ_{15}	.0169100
ζ_{16}	57.104373	.3607767	-.1859413	.0510743	ζ_{16}	.0545733
ζ_{17}	29.952163	.3399990	-.1176673	.0286115	ζ_{17}	.1385786
ζ_{18}	15.762483	.1375085	.1921627	-.0686855	ζ_{18}	.2503782
ζ_{19}	8.3119034	.0200484	.4426426	-.1462124	ζ_{19}	.3138473
ζ_{20}	4.3882382	.0010890	.3744549	-.1131994	ζ_{20}	.2875366
ζ_{21}	2.3182716	.0003687	.1331056	.0664730	ζ_{21}	.1885353
ζ_{22}	1.2251404	-.0000939	.0190403	.2722450	ζ_{22}	.0792933
ζ_{23}	0.6475567	.0000796	.0008536	.3567720	ζ_{23}	.0262106
ζ_{24}	.34229458	-.0000483	.0002775	.3073438		
ζ_{25}	.18093959	.0000222	-.0001491	.1573280		
ζ_{26}	.09564686	-.0000068	.0000260	.0613467		

Table 76. Os ^{5}D (28s, 21p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	21	18	12
Nuclear charge	76	Number of closed shells	6	4	2	1
No. of electrons	76	Open-shell occupation	0	0	6	0

Coupling coefficients

$K_0^{dd} = -0.13333333 \quad K_2^{dd} = -0.02222222 \quad K_4^{dd} = -0.02222222$

Total energy	Potential energy	Kinetic energy	Virial theorem
-16290.64760	-32581.29920	16290.65160	-1.99999975

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2497.64580	-418.40960	-98.71525	-21.50008	-3.33344	-0.23869
ζ_1	91549282.	.0000024	-.0000008	.0000004	-.0000002	.0000001	.0000000
ζ_2	18522020.	.0000137	-.0000045	.0000021	-.0000011	.0000004	-.0000001
ζ_3	4348043.2	.0000778	-.0000259	.0000122	-.0000060	.0000025	-.0000006
ζ_4	1171256.9	.0003605	-.0001198	.0000566	-.0000278	.0000113	-.0000030
ζ_5	357424.64	.0014368	-.0004785	.0002259	-.0001111	.0000454	-.0000119
ζ_6	121823.62	.0049717	-.0016611	.0007846	-.0003852	.0001574	-.0000412
ζ_7	45688.233	.0151829	-.0051230	.0024237	-.0011926	.0004878	-.0001277
ζ_8	18572.772	.0411449	-.0141797	.0067292	-.0033064	.0013505	-.0003534
ζ_9	8066.3284	.0980921	-.0354683	.0169604	-.0083716	.0034283	-.0008977
ζ_{10}	3693.4349	.1980086	-.0787507	.0382137	-.0188602	.0077076	-.0020168
ζ_{11}	1762.1595	.3100818	-.1487826	.0744645	-.0372119	.0152935	-.0040077
ζ_{12}	867.34575	.3133493	-.2056770	.1088286	-.0546771	.0223978	-.0058607
ζ_{13}	436.84215	.1466443	-.1112500	.0648105	-.0343478	.0144439	-.0038060
ζ_{14}	223.68158	.0169120	.2806823	-.2071409	.1151416	-.0487794	.0128589
ζ_{15}	115.86415	.0011221	.5886872	-.6052701	.3558382	-.1507402	.0396280
ζ_{16}	60.488245	-.0006781	.3048771	-.3589925	.2527536	-.1149263	.0306740
ζ_{17}	31.741786	.0004602	.0274388	.6943109	-.6909692	.3383119	-.0912550
ζ_{18}	16.711433	-.0003896	.0025780	.6772731	-.9218339	.4643641	-.1250951
ζ_{19}	8.8158517	.0002924	-.0017639	.0917455	.3978705	-.2374500	.0641073
ζ_{20}	4.6560883	-.0002079	.0010269	.0165073	.9184252	-.8650086	.2640745
ζ_{21}	2.4606951	.0001517	-.0007905	-.0086203	.2686624	-.3491448	.1048525
ζ_{22}	1.3008853	-.0001083	.0005694	.0064396	.0056778	.6590278	-.2464830
ζ_{23}	0.6878426	.0000753	-.0003884	-.0047607	.0061040	.6609662	-.3431522
ζ_{24}	.36372127	-.0000506	.0002639	.0032114	-.0026184	.1921953	-.1896112
ζ_{25}	.19233546	.0000318	-.0001657	-.0020492	.0017721	.0021295	.0883206
ζ_{26}	.10170760	-.0000175	.0000916	.0011387	-.0009532	.0053714	.4327709
ζ_{27}	.05378340	.0000074	-.0000390	-.0004867	.0004059	-.0021720	.4577548
ζ_{28}	.02844089	-.0000018	.0000093	.0001162	-.0000968	.0005295	.2559272

Table 76. Os ^{5}D (28s, 21p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-400.96117	-90.54353	-17.98160	-2.17020
ζ_5	357424.64	.0000089	-.0000045	.0000022	-.0000008
ζ_6	121823.62	.0000417	-.0000208	.0000101	-.0000038
ζ_7	45688.233	.0002222	-.0001115	.0000541	-.0000205
ζ_8	18572.772	.0009669	-.0004840	.0002356	-.0000892
ζ_9	8066.3284	.0037747	-.0019060	.0009272	-.0003507
ζ_{10}	3693.4349	.0131328	-.0066769	.0032609	-.0012351
ζ_{11}	1762.1595	.0406037	-.0211209	.0103489	-.0039204
ζ_{12}	867.34575	.1085835	-.0584511	.0289269	-.0109863
ζ_{13}	436.84215	.2333978	-.1334381	.0668877	-.0254622
ζ_{14}	223.68158	.3571495	-.2181321	.1116435	-.0427113
ζ_{15}	115.86415	.3052522	-.1529304	.0719985	-.0269836
ζ_{16}	60.488245	.1034772	.2328464	-.1788727	.0739997
ζ_{17}	31.741786	.0076824	.5708562	-.4693259	.1986702
ζ_{18}	16.711433	.0004004	.3129478	-.1273529	.0349645
ζ_{19}	8.8158517	-.0002943	.0417183	.5261050	-.2965583
ζ_{20}	4.6560883	.0000830	.0038225	.5452394	-.3728544
ζ_{21}	2.4606951	-.0000733	-.0009569	.1451920	.0623782
ζ_{22}	1.3008853	.0000463	.0006871	.0099502	.4922172
ζ_{23}	0.6878426	-.0000237	-.0004406	.0006710	.4586154
ζ_{24}	.36372127	.0000114	.0001889	.0002097	.1631654
ζ_{25}	.19233546	-.0000029	-.0000523	-.0000622	.0294063

	Orbital	3d	4d	5d		4f
	Energy	-75.50526	-11.57715	-0.53563		-3.05897
ζ_9	8066.3284	.0000969	-.0000481	.0000136		
ζ_{10}	3693.4349	.0003563	-.0001809	.0000516		
ζ_{11}	1762.1595	.0018423	-.0009205	.0002597		
ζ_{12}	867.34575	.0077538	-.0039463	.0011228	ζ_{12}	.0001869
ζ_{13}	436.84215	.0286990	-.0146216	.0041461	ζ_{13}	.0007664
ζ_{14}	223.68158	.0892342	-.0465623	.0132908	ζ_{14}	.0039166
ζ_{15}	115.86415	.2137182	-.1129557	.0322336	ζ_{15}	.0165026
ζ_{16}	60.488245	.3571138	-.1859571	.0531134	ζ_{16}	.0538240
ζ_{17}	31.741786	.3454733	-.1257366	.0321919	ζ_{17}	.1379585
ζ_{18}	16.711433	.1449233	.1809830	-.0682924	ζ_{18}	.2518707
ζ_{19}	8.8158517	.0218206	.4426165	-.1530260	ζ_{19}	.3176743
ζ_{20}	4.6560883	.0012564	.3817340	-.1213316	ζ_{20}	.2899960
ζ_{21}	2.4606951	.0003081	.1356562	.0723803	ζ_{21}	.1843472
ζ_{22}	1.3008853	-.0000569	.0190084	.2853217	ζ_{22}	.0736387
ζ_{23}	0.6878426	.0000485	.0009422	.3573295	ζ_{23}	.0218615
ζ_{24}	.36372127	-.0000329	.0003485	.2989085		
ζ_{25}	.19233546	.0000132	-.0000918	.1511576		
ζ_{26}	.10170760	-.0000047	.0000416	.0598204		

Table 77. Ir ^{4}F (28s, 21p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	21	18	12
Nuclear charge	77	Number of closed shells	6	4	2	1
No. of electrons	77	Open-shell occupation	0	0	7	0

Coupling coefficients

$K_0^{dd} = -0.08571429$ $K_2^{dd} = -0.01449396$ $K_4^{dd} = -0.00283215$

Total energy	Potential energy	Kinetic energy	Virial theorem
-16806.11218	-33612.22920	16806.11700	-1.99999971

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2566.48430	-431.19186	-102.22146	-22.48913	-3.54460	-0.24528
ζ_1	94689771.	.0000024	-.0000008	.0000004	-.0000002	.0000001	.0000000
ζ_2	19312937.	.0000133	-.0000044	.0000021	-.0000010	.0000004	-.0000001
ζ_3	4555994.7	.0000756	-.0000252	.0000119	-.0000059	.0000024	-.0000006
ζ_4	1230017.6	.0003501	-.0001165	.0000550	-.0000271	.0000112	-.0000029
ζ_5	375413.98	.0013973	-.0004656	.0002202	-.0001086	.0000450	-.0000118
ζ_6	127789.30	.0048491	-.0016210	.0007668	-.0003779	.0001564	-.0000408
ζ_7	47823.634	.0148643	-.0050176	.0023774	-.0011740	.0004865	-.0001271
ζ_8	19394.076	.0404430	-.0139394	.0066243	-.0032668	.0013518	-.0003529
ζ_9	8404.2078	.0967965	-.0349823	.0167520	-.0082978	.0034427	-.0008995
ζ_{10}	3841.4461	.1961801	-.0779103	.0378491	-.0187490	.0077623	-.0020264
ζ_{11}	1830.8483	.3087664	-.1476690	.0739896	-.0371007	.0154487	-.0040397
ζ_{12}	900.90061	.3147292	-.2055138	.1087814	-.0548582	.0227650	-.0059424
ζ_{13}	453.96052	.1498111	-.1152291	.0672043	-.0356756	.0151983	-.0039979
ζ_{14}	232.72071	.0179592	.2710537	-.1997776	.1113763	-.0478460	.0125935
ζ_{15}	120.76021	.0011356	.5870429	-.5999648	.3537271	-.1517829	.0398050
ζ_{16}	63.186663	-.0006731	.3140583	-.3779093	.2657356	-.1223832	.0326227
ζ_{17}	33.245073	.0004635	.0301466	.6726576	-.6677964	.3317659	-.0894304
ζ_{18}	17.553763	-.0003962	.0026337	.6938285	-.9451491	.4829362	-.1298436
ζ_{19}	9.2889135	.0002985	-.0017943	.1011551	.3582851	-.2144049	.0572924
ζ_{20}	4.9217725	-.0002130	.0010596	.0169285	.9332486	-.8889949	.2720629
ζ_{21}	2.6097127	.0001560	-.0008231	-.0086802	.2848305	-.3732382	.1112002
ζ_{22}	1.3842960	-.0001117	.0005955	.0065267	.0065977	.6648410	-.2495000
ζ_{23}	0.7344211	.0000777	-.0004072	-.0048534	.0065722	.6645652	-.3434507
ζ_{24}	.38966943	-.0000524	.0002769	.0032791	-.0028262	.1980151	-.1835918
ζ_{25}	.20675729	.0000329	-.0001739	-.0020944	.0019180	.0021448	.0721756
ζ_{26}	.10970579	-.0000181	.0000959	.0011631	-.0010296	.0059133	.4273495
ζ_{27}	.05821023	.0000077	-.0000407	-.0004961	.0004376	-.0023932	.4396078
ζ_{28}	.03088653	-.0000018	.0000097	.0001180	-.0001040	.0005830	.2890552

Table 77. Ir ^{4}F (28s, 21p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-413.46789	-93.89478	-18.88271	-2.33842
ζ_5	375413.98	.0000086	-.0000043	.0000021	-.0000008
ζ_6	127789.30	.0000403	-.0000201	.0000098	-.0000038
ζ_7	47823.634	.0002156	-.0001083	.0000528	-.0000203
ζ_8	19394.076	.0009426	-.0004728	.0002312	-.0000890
ζ_9	8404.2078	.0036946	-.0018686	.0009130	-.0003510
ζ_{10}	3841.4461	.0128957	-.0065689	.0032225	-.0012411
ζ_{11}	1830.8483	.0399580	-.0208146	.0102433	-.0039448
ζ_{12}	900.90061	.1070583	-.0577166	.0286900	-.0110798
ζ_{13}	453.96052	.2307429	-.1320462	.0664757	-.0257270
ζ_{14}	232.72071	.3551895	-.2173012	.1117301	-.0434722
ζ_{15}	120.76021	.3077765	-.1570649	.0748171	-.0285430
ζ_{16}	63.186663	.1072120	.2217726	-.1721520	.0725134
ζ_{17}	33.245073	.0083846	.5681897	-.4689866	.2021968
ζ_{18}	17.553763	.0004332	.3227472	-.1454111	.0441671
ζ_{19}	9.2889135	-.0003143	.0452111	.5153293	-.2966530
ζ_{20}	4.9217725	.0000966	.0040633	.5558263	-.3888209
ζ_{21}	2.6097127	-.0000839	-.0010276	.1518802	.0578850
ζ_{22}	1.3842960	.0000539	.0007312	.0106584	.4976680
ζ_{23}	0.7344211	-.0000276	-.0004767	.0007605	.4590263
ζ_{24}	.38966943	.0000133	.0002030	.0002223	.1631262
ζ_{25}	.20675729	-.0000033	-.0000565	-.0000553	.0296355

	Orbital	3d	4d	5d		4f
	Energy	-78.56922	-12.30860	-0.57383		-3.52145
ζ_9	8404.2078	.0000944	-.0000472	.0000138		
ζ_{10}	3841.4461	.0003493	-.0001785	.0000527		
ζ_{11}	1830.8483	.0018091	-.0009108	.0002662		
ζ_{12}	900.90061	.0076185	-.0039049	.0011509	ζ_{12}	.0001879
ζ_{13}	453.96052	.0282199	-.0144841	.0042544	ζ_{13}	.0007694
ζ_{14}	232.72071	.0877860	-.0461336	.0136429	ζ_{14}	.0039311
ζ_{15}	120.76021	.2108279	-.1122854	.0331987	ζ_{15}	.0165362
ζ_{16}	63.186663	.3543339	-.1861529	.0551035	ζ_{16}	.0539940
ζ_{17}	33.245073	.3471248	-.1298427	.0345976	ζ_{17}	.1384930
ζ_{18}	17.553763	.1491096	.1737732	-.0688005	ζ_{18}	.2533115
ζ_{19}	9.2889135	.0231757	.4413643	-.1591490	ζ_{19}	.3200102
ζ_{20}	4.9217725	.0013513	.3863596	-.1284466	ζ_{20}	.2905438
ζ_{21}	2.6097127	.0002900	.1375897	.0770575	ζ_{21}	.1797674
ζ_{22}	1.3842960	-.0000497	.0192537	.2951074	ζ_{22}	.0686733
ζ_{23}	0.7344211	.0000385	.0009953	.3578350	ζ_{23}	.0189478
ζ_{24}	.38966943	-.0000292	.0004271	.2925709		
ζ_{25}	.20675729	.0000104	-.0000666	.1455206		
ζ_{26}	.10970579	-.0000042	.0000557	.0576295		

Table 78. Pt ^{3}F (28s, 21p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	21	18	12
Nuclear charge	78	Number of closed shells	6	4	2	1
No. of electrons	78	Open-shell occupation	0	0	8	0

Coupling coefficients

$K_0^{dd} = -0.05000000$ $K_2^{dd} = -0.00663265$ $K_4^{dd} = 0.00229592$

Total energy	Potential energy	Kinetic energy	Virial theorem
-17330.94853	-34661.89750	17330.94900	-1.99999997

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2636.27011	-444.17415	-105.79447	-23.49830	-3.75643	-0.25113
ζ_1	97069151.	.0000024	-.0000008	.0000004	-.0000002	.0000001	.0000000
ζ_2	20323110.	.0000127	-.0000042	.0000020	-.0000010	.0000004	-.0000001
ζ_3	4876833.2	.0000711	-.0000237	.0000112	-.0000055	.0000023	-.0000006
ζ_4	1328855.7	.0003267	-.0001088	.0000515	-.0000255	.0000107	-.0000028
ζ_5	406753.55	.0013056	-.0004353	.0002061	-.0001021	.0000428	-.0000111
ζ_6	138201.16	.0045603	-.0015251	.0007224	-.0003573	.0001496	-.0000389
ζ_7	51463.823	.0141179	-.0047655	.0022612	-.0011205	.0004700	-.0001222
ζ_8	20733.411	.0388558	-.0133827	.0063674	-.0031515	.0013197	-.0003428
ζ_9	8922.7141	.0941066	-.0339406	.0162723	-.0080877	.0033958	-.0008830
ζ_{10}	4053.0081	.1929657	-.0763343	.0371086	-.0184488	.0077295	-.0020077
ζ_{11}	1922.1628	.3073737	-.1459941	.0731879	-.0368154	.0155140	-.0040378
ζ_{12}	942.75848	.3180202	-.2057502	.1088440	-.0550899	.0231346	-.0060072
ζ_{13}	474.36005	.1549604	-.1212604	.0707507	-.0375908	.0161992	-.0042454
ζ_{14}	243.24419	.0194975	.2579249	-.1895907	.1059612	-.0461149	.0120966
ζ_{15}	126.45004	.0011745	.5842915	-.5916049	.3495195	-.1517004	.0395593
ζ_{16}	66.369952	-.0006797	.3263852	-.4027282	.2823533	-.1315056	.0349519
ζ_{17}	35.064975	.0004806	.0343829	.6381903	-.6297744	.3170915	-.0852886
ζ_{18}	18.606197	-.0004167	.0026595	.7165026	-.9732970	.5033062	-.1344738
ζ_{19}	9.9001060	.0003163	-.0017748	.1168043	.2897463	-.1718510	.0445186
ζ_{20}	5.2765871	-.0002277	.0010619	.0177625	.9480392	-.9002228	.2754081
ζ_{21}	2.8150788	.0001680	-.0008412	-.0087029	.3187019	-.4288184	.1265005
ζ_{22}	1.5026560	-.0001209	.0006126	.0066450	.0082145	.6445847	-.2387759
ζ_{23}	0.8023168	.0000845	-.0004204	-.0049874	.0081340	.6804694	-.3463650
ζ_{24}	.42843613	-.0000572	.0002868	.0033781	-.0037114	.2213463	-.1799901
ζ_{25}	.22879584	.0000360	-.0001801	-.0021617	.0025259	.0037764	.0269002
ζ_{26}	.12218490	-.0000198	.0000992	.0011988	-.0013621	.0069162	.4251637
ζ_{27}	.06525126	.0000084	-.0000419	-.0005094	.0005783	-.0027842	.3963492
ζ_{28}	.03484661	-.0000020	.0000099	.0001204	-.0001368	.0006768	.3636859

Table 78. Pt ^{3}F (28s, 21p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-426.17395	-97.31211	-19.80320	-2.50796
ζ_5	406753.55	.0000078	-.0000039	.0000019	-.0000007
ζ_6	138201.16	.0000370	-.0000185	.0000091	-.0000036
ζ_7	51463.823	.0001999	-.0001006	.0000492	-.0000192
ζ_8	20733.411	.0008864	-.0004456	.0002189	-.0000856
ζ_9	8922.7141	.0035202	-.0017826	.0008746	-.0003413
ζ_{10}	4053.0081	.0124300	-.0063427	.0031253	-.0012223
ζ_{11}	1922.1628	.0388590	-.0202590	.0100113	-.0039131
ζ_{12}	942.75848	.1048194	-.0565691	.0282416	-.0110752
ζ_{13}	474.36005	.2272648	-.1300774	.0657492	-.0258264
ζ_{14}	243.24419	.3527842	-.2161270	.1116337	-.0441177
ζ_{15}	126.45004	.3111870	-.1624395	.0783994	-.0303929
ζ_{16}	66.369952	.1124352	.2056829	-.1616880	.0691964
ζ_{17}	35.064975	.0095150	.5626083	-.4657936	.2043067
ζ_{18}	18.606197	.0004653	.3372361	-.1724391	.0579766
ζ_{19}	9.9001060	-.0003258	.0512195	.4926073	-.2885289
ζ_{20}	5.2765871	.0001037	.0045142	.5710079	-.4065723
ζ_{21}	2.8150788	-.0000916	-.0011004	.1673416	.0354459
ζ_{22}	1.5026560	.0000596	.0007917	.0122945	.4918692
ζ_{23}	0.8023168	-.0000304	-.0005248	.0011325	.4673062
ζ_{24}	.42843613	.0000148	.0002214	.0001479	.1733491
ζ_{25}	.22879584	-.0000036	-.0000620	-.0000193	.0334574

	Orbital	3d	4d	5d		4f
	Energy	-81.69792	-13.05831	-0.61575		-4.00165
ζ_9	8922.7141	.0000882	-.0000445	.0000134		
ζ_{10}	4053.0081	.0003344	-.0001719	.0000524		
ζ_{11}	1922.1628	.0017429	-.0008843	.0002668		
ζ_{12}	942.75848	.0073917	-.0038134	.0011599	ζ_{12}	.0001849
ζ_{13}	474.36005	.0275007	-.0142185	.0043113	ζ_{13}	.0007624
ζ_{14}	243.24419	.0857094	-.0453415	.0138398	ζ_{14}	.0038946
ζ_{15}	126.45004	.2065996	-.1108676	.0338436	ζ_{15}	.0163560
ζ_{16}	66.369952	.3497793	-.1854258	.0566766	ζ_{16}	.0534283
ζ_{17}	35.064975	.3491834	-.1356968	.0376829	ζ_{17}	.1370982
ζ_{18}	18.606197	.1558010	.1604898	-.0668230	ζ_{18}	.2518969
ζ_{19}	9.9001060	.0256283	.4353917	-.1631152	ζ_{19}	.3202896
ζ_{20}	5.2765871	.0015526	.3941494	-.1376867	ζ_{20}	.2915351
ζ_{21}	2.8150788	.0002788	.1450933	.0729493	ζ_{21}	.1785483
ζ_{22}	1.5026560	-.0000379	.0210260	.2973268	ζ_{22}	.0665559
ζ_{23}	0.8023168	.0000260	.0012719	.3566576	ζ_{23}	.0179704
ζ_{24}	.42843613	-.0000247	.0004945	.2920607		
ζ_{25}	.22879584	.0000066	-.0000114	.1445666		
ζ_{26}	.12218490	-.0000036	.0000691	.0606909		

Table 79. Au ^{2}D (28s, 21p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	21	18	12
Nuclear charge	79	Number of closed shells	6	4	2	1
No. of electrons	79	Open-shell occupation	0	0	9	0

Coupling coefficients

$K_0^{dd} = -0.02222222$ $K_2^{dd} = 0.00070547$ $K_4^{dd} = 0.00070547$

Total energy	Potential energy	Kinetic energy	Virial theorem
-17865.21057	-35730.42490	17865.21430	-1.99999979

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2707.00293	-457.35613	-109.43380	-24.52730	-3.96944	-0.25645
ζ_1	103551660.	.0000023	-.0000008	.0000004	-.0000002	.0000001	.0000000
ζ_2	21175219.	.0000126	-.0000042	.0000020	-.0000010	.0000004	-.0000001
ζ_3	5001590.6	.0000717	-.0000239	.0000113	-.0000056	.0000024	-.0000006
ζ_4	1350617.9	.0003322	-.0001106	.0000524	-.0000260	.0000110	-.0000028
ζ_5	412024.29	.0013275	-.0004429	.0002100	-.0001044	.0000443	-.0000114
ζ_6	140132.85	.0046144	-.0015443	.0007325	-.0003636	.0001539	-.0000397
ζ_7	52396.338	.0141708	-.0047871	.0022750	-.0011314	.0004798	-.0001239
ζ_8	21234.288	.0386461	-.0133201	.0063462	-.0031522	.0013344	-.0003442
ζ_9	9199.4532	.0928268	-.0334896	.0160808	-.0080217	.0034059	-.0008796
ζ_{10}	4206.2952	.1894683	-.0748604	.0364293	-.0181739	.0076967	-.0019851
ζ_{11}	2006.6241	.3026299	-.1430354	.0717658	-.0362275	.0154396	-.0039911
ζ_{12}	988.93492	.3184332	-.2037990	.1077071	-.0546839	.0232060	-.0059832
ζ_{13}	499.38454	.1614555	-.1288551	.0751171	-.0399686	.0174189	-.0045337
ζ_{14}	256.68227	.0221216	.2374045	-.1734976	.0972264	-.0428678	.0111766
ζ_{15}	133.60092	.0011875	.5812770	-.5798806	.3426898	-.1501951	.0388880
ζ_{16}	70.142211	-.0006334	.3450316	-.4360289	.3043792	-.1431320	.0377728
ζ_{17}	37.038981	.0004545	.0395778	.6041861	-.5924924	.3020354	-.0807716
ζ_{18}	19.631762	-.0004008	.0028712	.7418800	-.0047977	.5255510	-.1395670
ζ_{19}	10.429578	.0003038	-.0019116	.1289113	.2474985	-.1456148	.0368869
ζ_{20}	5.5484649	-.0002180	.0011847	.0185891	.9656956	-.9280941	.2827285
ζ_{21}	2.9540414	.0001606	-.0009426	-.0090081	.3301633	-.4427479	.1293763
ζ_{22}	1.5733993	-.0001154	.0006890	.0068926	.0085132	.6653708	-.2473025
ζ_{23}	0.8382019	.0000805	-.0004747	-.0051866	.0083702	.6779689	-.3432631
ζ_{24}	.44657751	-.0000543	.0003239	.0035173	-.0037810	.2156426	-.1732943
ζ_{25}	.23793590	.0000341	-.0002036	-.0022524	.0025637	.0020294	.0315571
ζ_{26}	.12677333	-.0000188	.0001123	.0012506	-.0013805	.0073055	.4228725
ζ_{27}	.06754559	.0000080	-.0000476	-.0005323	.0005863	-.0029793	.3927553
ζ_{28}	.03598871	-.0000019	.0000112	.0001262	-.0001389	.0007260	.3637999

Table 79. Au ^{2}D (28s, 21p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-439.07900	-100.79506	-20.74284	-2.67927
ζ_5	412024.29	.0000080	-.0000040	.0000020	-.0000008
ζ_6	140132.85	.0000377	-.0000189	.0000093	-.0000037
ζ_7	52396.338	.0002017	-.0001016	.0000500	-.0000197
ζ_8	21234.288	.0008834	-.0004450	.0002197	-.0000871
ζ_9	9199.4532	.0034654	-.0017576	.0008658	-.0003424
ζ_{10}	4206.2952	.0121116	-.0061915	.0030650	-.0012157
ζ_{11}	2006.6241	.0375969	-.0196232	.0097358	-.0038574
ζ_{12}	988.93492	.1012795	-.0546972	.0274269	-.0109074
ζ_{13}	499.38454	.2208799	-.1263522	.0640991	-.0255220
ζ_{14}	256.68227	.3486389	-.2136497	.1108389	-.0444279
ζ_{15}	133.60092	.3173379	-.1707386	.0837114	-.0329800
ζ_{16}	70.142211	.1203943	.1859952	-.1486709	.0646193
ζ_{17}	37.038981	.0109102	.5602388	-.4649965	.2070767
ζ_{18}	19.631762	.0005530	.3529719	-.1970266	.0708984
ζ_{19}	10.429578	-.0003828	.0556936	.4833219	-.2884982
ζ_{20}	5.5484649	.0001455	.0049972	.5833147	-.4232092
ζ_{21}	2.9540414	-.0001221	-.0013343	.1716955	.0371985
ζ_{22}	1.5733993	.0000805	.0009404	.0123812	.5046951
ζ_{23}	0.8382019	-.0000421	-.0006240	.0012168	.4643790
ζ_{24}	.44657751	.0000203	.0002657	.0001427	.1674780
ζ_{25}	.23793590	-.0000051	-.0000744	-.0000108	.0306446

	Orbital	3d	4d	5d		4f
	Energy	-84.89090	-13.82615	-0.66059		-4.49948
ζ_9	9199.4532	.0000877	-.0000445	.0000138		
ζ_{10}	4206.2952	.0003237	-.0001675	.0000525		
ζ_{11}	2006.6241	.0016792	-.0008580	.0002665		
ζ_{12}	988.93492	.0070606	-.0036664	.0011481	ζ_{12}	.0001797
ζ_{13}	499.38454	.0262657	-.0136723	.0042680	ζ_{13}	.0007349
ζ_{14}	256.68227	.0822631	-.0437859	.0137591	ζ_{14}	.0037583
ζ_{15}	133.60092	.2007373	-.1084877	.0341020	ζ_{15}	.0158854
ζ_{16}	70.142211	.3460413	-.1851673	.0582973	ζ_{16}	.0524985
ζ_{17}	37.038981	.3542400	-.1429095	.0412537	ζ_{17}	.1363100
ζ_{18}	19.631762	.1630429	.1507767	-.0658102	ζ_{18}	.2534230
ζ_{19}	10.429578	.0274117	.4366561	-.1694575	ζ_{19}	.3244641
ζ_{20}	5.5484649	.0017216	.4005112	-.1450079	ζ_{20}	.2938794
ζ_{21}	2.9540414	.0002079	.1456956	.0803206	ζ_{21}	.1744142
ζ_{22}	1.5733993	.0000022	.0205381	.3100919	ζ_{22}	.0618198
ζ_{23}	0.8382019	-.0000102	.0013820	.3603073	ζ_{23}	.0152640
ζ_{24}	.44657751	-.0000084	.0006120	.2842069		
ζ_{25}	.23793590	-.0000039	.0000532	.1369651		
ζ_{26}	.12677333	-.0000014	.0000891	.0532472		

Table 80. Hg ^{1}S (29s, 21p, 19d, 13f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	29	21	19	13
Nuclear charge	80	Number of closed shells	6	4	3	1
No. of electrons	80	Open-shell occupation	0	0	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-18408.99066	-36817.97830	18408.98760	-2.00000017

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2778.68001	-470.73499	-113.13653	-25.57329	-4.18193	-0.26100
ζ_1	96293620.	.0000026	-.0000009	.0000004	-.0000002	.0000001	.0000000
ζ_2	19555636.	.0000145	-.0000048	.0000023	-.0000011	.0000005	-.0000001
ζ_3	4607673.0	.0000821	-.0000273	.0000130	-.0000065	.0000028	-.0000007
ζ_4	1245720.3	.0003784	-.0001261	.0000599	-.0000298	.0000128	-.0000033
ζ_5	381541.53	.0015007	-.0005011	.0002380	-.0001187	.0000508	-.0000130
ζ_6	130537.13	.0051643	-.0017304	.0008221	-.0004096	.0001752	-.0000448
ζ_7	49154.827	.0156716	-.0053044	.0025245	-.0012599	.0005396	-.0001379
ζ_8	20071.127	.0421529	-.0145815	.0069614	-.0034710	.0014845	-.0003793
ζ_9	8760.5591	.0995980	-.0361741	.0174072	-.0087148	.0037369	-.0009553
ζ_{10}	4033.8159	.1990133	-.0796073	.0388794	-.0194789	.0083361	-.0021300
ζ_{11}	1936.6618	.3084816	-.1489337	.0750682	-.0380538	.0163794	-.0041900
ζ_{12}	959.89580	.3099802	-.2044239	.1089213	-.0556063	.0238597	-.0060985
ζ_{13}	487.15958	.1463864	-.1117666	.0656168	-.0351810	.0155027	-.0039838
ζ_{14}	251.51405	.0177702	.2698175	-.2005323	.1130102	-.0502220	.0129216
ζ_{15}	131.43382	.0010839	.5821500	-.5980483	.3577617	-.1590033	.0408769
ζ_{16}	69.256611	-.0006261	.3177792	-.3872406	.2745300	-.1308915	.0340869
ζ_{17}	36.696456	.0004297	.0323527	.6559764	-.6588698	.3400957	-.0897435
ζ_{18}	19.513920	-.0003723	.0026016	.7045519	-.9717650	.5170798	-.1369436
ζ_{19}	10.400087	.0002821	-.0017697	.1124737	.3255624	-.1992317	.0527238
ζ_{20}	5.5502436	-.0002021	.0010539	.0163701	.9604131	-.9732235	.2938866
ζ_{21}	2.9642867	.0001495	-.0008296	-.0081695	.2893237	-.3626685	.1048564
ζ_{22}	1.5838295	-.0001085	.0006113	.0061944	.0099435	.7104556	-.2727491
ζ_{23}	0.8464232	.0000771	-.0004270	-.0047521	.0050955	.6490500	-.3178396
ζ_{24}	.45238567	-.0000539	.0003015	.0033327	-.0016526	.1911213	-.1837836
ζ_{25}	.24179521	.0000363	-.0002028	-.0022818	.0012461	-.0002513	.0917937
ζ_{26}	.12923879	-.0000228	.0001274	.0014439	-.0007284	.0080152	.3452583
ζ_{27}	.06907803	.0000125	-.0000700	-.0007977	.0003949	-.0043043	.4833509
ζ_{28}	.03692219	-.0000053	.0000296	.0003378	-.0001656	.0018710	.2728927
ζ_{29}	.01973490	.0000012	-.0000070	-.0000797	.0000389	-.0004501	.0383278

Table 80. Hg ^{1}S (29s, 21p, 19d, 13f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p
	Energy	-452.18026	-104.34071	-21.69884	-2.85080
ζ_5	381541.53	.0000095	-.0000048	.0000024	-.0000010
ζ_6	130537.13	.0000442	-.0000222	.0000110	-.0000044
ζ_7	49154.827	.0002342	-.0001183	.0000585	-.0000234
ζ_8	20071.127	.0010090	-.0005090	.0002520	-.0001010
ζ_9	8760.5591	.0039009	-.0019844	.0009830	-.0003941
ζ_{10}	4033.8159	.0134163	-.0068759	.0034162	-.0013709
ζ_{11}	1936.6618	.0409911	-.0214936	.0107252	-.0043074
ζ_{12}	959.89580	.1083074	-.0587971	.0296150	-.0119199
ζ_{13}	487.15958	.2306910	-.1329898	.0679213	-.0274216
ζ_{14}	251.51405	.3522207	-.2169454	.1130487	-.0458503
ζ_{15}	131.43382	.3055830	-.1571529	.0760759	-.0303115
ζ_{16}	69.256611	.1084076	.2167781	-.1724055	.0762016
ζ_{17}	36.696456	.0088575	.5639545	-.4727700	.2132053
ζ_{18}	19.513920	.0004523	.3285885	-.1592973	.0531851
ζ_{19}	10.400087	-.0003343	.0488715	.5127863	-.3140577
ζ_{20}	5.5502436	.0001103	.0038996	.5669265	-.4226496
ζ_{21}	2.9642867	-.0000920	-.0009213	.1501359	.0847702
ζ_{22}	1.5838295	.0000619	.0006100	.0117361	.5214534
ζ_{23}	0.8464232	-.0000309	-.0004315	.0002578	.4451722
ζ_{24}	.45238567	.0000152	.0001749	.0005628	.1498072
ζ_{25}	.24179521	-.0000037	-.0000500	-.0001237	.0261519

	Orbital	3d	4d	5d		4f
	Energy	-88.14530	-14.60953	-0.71413		-5.01230
ζ_8	20071.127	.0000170	-.0000089	.0000029		
ζ_9	8760.5591	.0000715	-.0000361	.0000113		
ζ_{10}	4033.8159	.0004143	-.0002166	.0000696		
ζ_{11}	1936.6618	.0018617	-.0009563	.0003027	ζ_{11}	.0000357
ζ_{12}	959.89580	.0079409	-.0041615	.0013322	ζ_{12}	.0001470
ζ_{13}	487.15958	.0287524	-.0150780	.0048033	ζ_{13}	.0009301
ζ_{14}	251.51405	.0885042	-.0475739	.0152817	ζ_{14}	.0042069
ζ_{15}	131.43382	.2103887	-.1145584	.0367602	ζ_{15}	.0178309
ζ_{16}	69.256611	.3520941	-.1892995	.0608878	ζ_{16}	.0573004
ζ_{17}	36.696456	.3449174	-.1313042	.0375230	ζ_{17}	.1458127
ζ_{18}	19.513920	.1501559	.1738617	-.0761503	ζ_{18}	.2628195
ζ_{19}	10.400087	.0239542	.4469687	-.1784907	ζ_{19}	.3278816
ζ_{20}	5.5502436	.0013029	.3870963	-.1392703	ζ_{20}	.2863380
ζ_{21}	2.9642867	.0002803	.1294407	.1072222	ζ_{21}	.1596574
ζ_{22}	1.5838295	-.0000697	.0172554	.3269950	ζ_{22}	.0526540
ζ_{23}	0.8464232	.0000492	.0003718	.3588823	ζ_{23}	.0117324
ζ_{24}	.45238567	-.0000305	.0005169	.2682938		
ζ_{25}	.24179521	.0000143	-.0002178	.1242068		
ζ_{26}	.12923879	-.0000041	.0000651	.0436812		

Table 81. Tl ^{2}P (28s, 24p, 18d, 12f; 29 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	24	18	12
Nuclear charge	81	Number of closed shells	6	4	3	1
No. of electrons	81	Open-shell occupation	0	1	0	0

Coupling coefficients

$K_0^{pp} = -1.66666667$ $K_2^{pp} = 0.13333333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-18961.82286	-37923.65060	18961.82770	-1.99999975

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2851.54652	-484.55970	-117.15001	-26.88302	-4.61852	-0.36102
ζ_1	109459110.	.0000023	-.0000008	.0000004	-.0000002	.0000001	.0000000
ζ_2	22248380.	.0000128	-.0000043	.0000020	-.0000010	.0000004	-.0000001
ζ_3	5181281.8	.0000740	-.0000247	.0000117	-.0000059	.0000025	-.0000007
ζ_4	1370380.7	.0003539	-.0001180	.0000561	-.0000281	.0000122	-.0000035
ζ_5	407442.84	.0014678	-.0004903	.0002331	-.0001166	.0000506	-.0000145
ζ_6	134635.49	.0053086	-.0017801	.0008474	-.0004240	.0001843	-.0000529
ζ_7	48844.324	.0169366	-.0057379	.0027329	-.0013674	.0005937	-.0001703
ζ_8	19211.864	.0476211	-.0165318	.0079140	-.0039653	.0017246	-.0004949
ζ_9	8091.3614	.1159787	-.0425310	.0205009	-.0102875	.0044682	-.0012812
ζ_{10}	3605.9814	.2318901	-.0953203	.0468917	-.0236527	.0103095	-.0029598
ζ_{11}	1682.0961	.3395378	-.1743268	.0887168	-.0451119	.0196361	-.0056313
ζ_{12}	813.42314	.2880205	-.2105624	.1154637	-.0598508	.0263321	-.0075774
ζ_{13}	404.41800	.0941112	-.0215388	.0106143	-.0054551	.0021124	-.0005730
ζ_{14}	205.30914	.0052417	.4403288	-.3584784	.2048696	-.0912240	.0262329
ζ_{15}	105.83779	.0005321	.5543849	-.6637262	.4213865	-.1958022	.0569480
ζ_{16}	55.161591	-.0002988	.1673454	.0117615	-.0220382	.0152390	-.0049565
ζ_{17}	28.970233	.0001110	.0071742	.8872827	-.0289063	.5416267	-.1601152
ζ_{18}	15.293723	-.0000833	-.0002443	.4069497	-.5212309	.3050103	-.0941274
ζ_{19}	8.1011289	.0000627	.0003074	.0368910	.8460601	-.6620366	.2145424
ζ_{20}	4.3003763	-.0000396	-.0005384	-.0005191	.7128192	-.9317452	.3260584
ζ_{21}	2.2857507	.0000286	.0004424	.0018601	.0631286	.2837654	-.1325768
ζ_{22}	1.2158331	-.0000213	-.0003293	-.0018288	.0205796	.8247596	-.3901868
ζ_{23}	0.6469838	.0000153	.0002500	.0012718	-.0110401	.4106205	-.3371443
ζ_{24}	.34434999	-.0000108	-.0001752	-.0009212	.0082751	.0290557	-.0014565
ζ_{25}	.18329320	.0000071	.0001147	.0005937	-.0052670	.0102383	.3593171
ζ_{26}	.09756822	-.0000040	-.0000654	-.0003323	.0029488	-.0050742	.5250586
ζ_{27}	.05193686	.0000018	.0000285	.0001425	-.0012671	.0023087	.3013048
ζ_{28}	.02764677	-.0000004	-.0000069	-.0000339	.0003015	-.0005486	.0488002
ζ_{29}	.01471679						

Table 81. Tl ^{2}P (28s, 24p, 18d, 12f; 29 ζ) (continued)

	Orbital	2p	3p	4p	5p	6p
	Energy	-465.72623	-108.19633	-22.91727	-3.23113	-0.19231
ζ_6	134635.49	.0000605	-.0000304	.0000151	-.0000061	.0000013
ζ_7	48844.324	.0002392	-.0001212	.0000605	-.0000249	.0000053
ζ_8	19211.864	.0012062	-.0006091	.0003016	-.0001228	.0000262
ζ_9	8091.3614	.0048415	-.0024717	.0012342	-.0005069	.0001085
ζ_{10}	3605.9814	.0174978	-.0090020	.0044807	-.0018280	.0003908
ζ_{11}	1682.0961	.0547325	-.0289726	.0145849	-.0059967	.0012841
ζ_{12}	813.42314	.1429938	-.0788031	.0398842	-.0163371	.0034944
ζ_{13}	404.41800	.2861486	-.1693053	.0876998	-.0363107	.0077833
ζ_{14}	205.30914	.3734403	-.2310926	.1203438	-.0494725	.0105835
ζ_{15}	105.83779	.2401816	-.0536369	.0120270	-.0040264	.0008496
ζ_{16}	55.161591	.0505463	.4138459	-.3307595	.1517237	-.0330093
ζ_{17}	28.970233	.0020861	.5363734	-.4482093	.2014872	-.0435665
ζ_{18}	15.293723	-.0003121	.1712524	.1589806	-.1110930	.0251505
ζ_{19}	8.1011289	.0001636	.0170209	.6536673	-.4501206	.1043280
ζ_{20}	4.3003763	-.0002141	-.0016681	.3762101	-.2531634	.0562081
ζ_{21}	2.2857507	.0001612	.0018030	.0411843	.3843910	-.1105487
ζ_{22}	1.2158331	-.0001119	-.0014832	.0089695	.5475770	-.1614511
ζ_{23}	0.6469838	.0000832	.0010282	-.0041920	.2918201	-.1040051
ζ_{24}	.34434999	-.0000571	-.0007435	.0032974	.0455238	.0442586
ζ_{25}	.18329320	.0000387	.0005044	-.0022617	.0093526	.2240972
ζ_{26}	.09756822	-.0000246	-.0003229	.0014520	-.0026213	.3707121
ζ_{27}	.05193686	.0000140	.0001846	-.0008409	.0021320	.3522267
ζ_{28}	.02764677	-.0000063	-.0000835	.0003813	-.0009089	.1553388
ζ_{29}	.01471679	.0000017	.0000219	-.0001007	.0002561	.0167489

	Orbital	3d	4d	5d		4f
	Energy	-91.70805	-15.65256	-0.96807		-5.78486
ζ_8	19211.864	.0000199	-.0000105	.0000036		
ζ_9	8091.3614	.0000970	-.0000494	.0000163		
ζ_{10}	3605.9814	.0005792	-.0003046	.0001029		
ζ_{11}	1682.0961	.0027806	-.0014410	.0004802	ζ_{11}	.0000545
ζ_{12}	813.42314	.0120909	-.0063903	.0021528	ζ_{12}	.0002751
ζ_{13}	404.41800	.0437009	-.0231856	.0077786	ζ_{13}	.0015996
ζ_{14}	205.30914	.1283526	-.0700339	.0237090	ζ_{14}	.0076058
ζ_{15}	105.83779	.2755004	-.1510397	.0509930	ζ_{15}	.0299636
ζ_{16}	55.161591	.3855798	-.1994689	.0669131	ζ_{16}	.0899640
ζ_{17}	28.970233	.2763862	-.0249476	-.0033721	ζ_{17}	.2026388
ζ_{18}	15.293723	.0768891	.3293190	-.1411924	ζ_{18}	.3102379
ζ_{19}	8.1011289	.0080276	.4732772	-.2005844	ζ_{19}	.3280109
ζ_{20}	4.3003763	-.0001848	.2658053	-.0405354	ζ_{20}	.2313762
ζ_{21}	2.2857507	.0005313	.0511400	.2595536	ζ_{21}	.0927866
ζ_{22}	1.2158331	-.0003336	.0057856	.3834795	ζ_{22}	.0267116
ζ_{23}	0.6469838	.0002003	-.0008829	.3344750		
ζ_{24}	.34434999	-.0000981	.0005789	.1603246		
ζ_{25}	.18329320	.0000286	-.0001796	.0612928		

Table 82. Pb ^{3}P (28s, 24p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	24	18	12
Nuclear charge	82	Number of closed shells	6	4	3	1
No. of electrons	82	Open-shell occupation	0	2	0	0

Coupling coefficients

$K_0^{pp} = -0.66666667$ $K_2^{pp} = -0.06666667$

Total energy	Potential energy	Kinetic energy	Virial theorem
-19524.00666	-39048.01600	19524.00930	-1.99999987

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-2925.36926	-498.59392	-121.23816	-28.21976	-5.05544	-0.45619
ζ_1	73753376.	.0000038	-.0000013	.0000006	-.0000003	.0000001	.0000000
ζ_2	14954702.	.0000216	-.0000072	.0000034	-.0000017	.0000008	-.0000002
ζ_3	3513435.8	.0001228	-.0000410	.0000195	-.0000098	.0000043	-.0000013
ζ_4	946395.27	.0005690	-.0001900	.0000905	-.0000454	.0000200	-.0000062
ζ_5	288721.33	.0022662	-.0007581	.0003609	-.0001811	.0000798	-.0000247
ζ_6	98410.317	.0078097	-.0026268	.0012526	-.0006292	.0002776	-.0000859
ζ_7	36939.135	.0235888	-.0080410	.0038381	-.0019270	.0008489	-.0002626
ζ_8	15047.312	.0623689	-.0219385	.0105383	-.0053036	.0023420	-.0007252
ζ_9	6558.3089	.1414068	-.0531743	.0257615	-.0129778	.0057183	-.0017688
ζ_{10}	3018.2805	.2591056	-.1115444	.0553757	-.0281064	.0124486	-.0038576
ζ_{11}	1449.6318	.3380395	-.1867823	.0963679	-.0492671	.0217487	-.0067268
ζ_{12}	719.29575	.2448084	-.1922131	.1078897	-.0566212	.0254139	-.0079045
ζ_{13}	365.66620	.0638439	.0499976	-.0362894	.0204286	-.0097017	.0030767
ζ_{14}	189.18575	.0028735	.4929365	-.4241981	.2457889	-.1111516	.0344810
ζ_{15}	99.098613	.0000291	.5037419	-.6334166	.4140172	-.1975543	.0622184
ζ_{16}	52.351400	.0000648	.1259684	.1566154	-.1472024	.0806449	-.0263621
ζ_{17}	27.812067	-.0001615	.0049899	.8822043	-.0683946	.5734790	-.1831326
ζ_{18}	14.828806	.0001271	-.0007761	.3376690	-.3785214	.2348344	-.0803104
ζ_{19}	7.9240379	-.0000935	.0006077	.0324038	.9041788	-.7600733	.2715349
ζ_{20}	4.2399181	.0000752	-.0007054	-.0040804	.6448676	-.8861439	.3359649
ζ_{21}	2.2703218	-.0000557	.0005538	.0042060	.0442983	.3940513	-.1901642
ζ_{22}	1.2161428	.0000398	-.0003987	-.0035602	.0210681	.8271186	-.4494426
ζ_{23}	0.6515723	-.0000282	.0002911	.0025111	-.0116706	.3622383	-.3636105
ζ_{24}	.34912095	.0000190	-.0001979	-.0017609	.0085132	.0108921	.0969397
ζ_{25}	.18706936	-.0000119	.0001251	.0011256	-.0054203	.0127113	.4619113
ζ_{26}	.10023829	.0000066	-.0000690	-.0006238	.0030041	-.0065398	.5171415
ζ_{27}	.05371130	-.0000028	.0000291	.0002648	-.0012838	.0029699	.2082733
ζ_{28}	.02878047	.0000006	-.0000068	-.0000624	.0003027	-.0006995	.0194031

Table 82. Pb ^{3}P (28s, 24p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p	6p
	Energy	-479.48116	-112.12617	-24.16222	-3.61059	-0.25567
ζ_5	288721.33	.0000170	-.0000086	.0000043	-.0000018	.0000004
ζ_6	98410.317	.0000793	-.0000400	.0000198	-.0000082	.0000020
ζ_7	36939.135	.0004222	-.0002143	.0001074	-.0000450	.0000112
ζ_8	15047.312	.0018111	-.0009178	.0004565	-.0001896	.0000470
ζ_9	6558.3089	.0069464	-.0035601	.0017863	-.0007479	.0001860
ζ_{10}	3018.2805	.0232824	-.0120617	.0060354	-.0025112	.0006236
ζ_{11}	1449.6318	.0681652	-.0364455	.0184656	-.0077449	.0019266
ζ_{12}	719.29575	.1652627	-.0923760	.0470839	-.0196758	.0048890
ζ_{13}	365.66620	.3050212	-.1834019	.0958530	-.0405206	.0100925
ζ_{14}	189.18575	.3598374	-.2205148	.1147122	-.0479764	.0119173
ζ_{15}	99.098613	.2048214	.0014606	-.0234626	.0115532	-.0029194
ζ_{16}	52.351400	.0367769	.4578940	-.3721077	.1748769	-.0442721
ζ_{17}	27.812067	.0014353	.4995464	-.4093911	.1854236	-.0465163
ζ_{18}	14.828806	-.0003705	.1407409	.2305190	-.1538393	.0404910
ζ_{19}	7.9240379	.0001802	.0137369	.6551579	-.4743904	.1291584
ζ_{20}	4.2399181	-.0002066	-.0019790	.3334628	-.2034109	.0500942
ζ_{21}	2.2703218	.0001550	.0018630	.0325832	.4339776	-.1465795
ζ_{22}	1.2161428	-.0001052	-.0015193	.0075683	.5443392	-.1948281
ζ_{23}	0.6515723	.0000770	.0010396	-.0034706	.2554344	-.1113844
ζ_{24}	.34912095	-.0000514	-.0007277	.0026124	.0306557	.1041763
ζ_{25}	.18706936	.0000329	.0004679	-.0017053	.0078822	.3164112
ζ_{26}	.10023829	-.0000187	-.0002674	.0009711	-.0022924	.4156438
ζ_{27}	.05371130	.0000084	.0001208	-.0004452	.0014490	.2669099
ζ_{28}	.02878047	-.0000022	-.0000315	.0001163	-.0003460	.0745744

	Orbital	3d	4d	5d		4f
	Energy	-95.34375	-16.72074	-1.22034		-6.58227
ζ_8	15047.312	.0000359	-.0000189	.0000067		
ζ_9	6558.3089	.0001563	-.0000809	.0000280		
ζ_{10}	3018.2805	.0008687	-.0004577	.0001611		
ζ_{11}	1449.6318	.0038917	-.0020397	.0007113	ζ_{11}	.0000877
ζ_{12}	719.29575	.0157173	-.0083613	.0029397	ζ_{12}	.0003974
ζ_{13}	365.66620	.0531886	-.0285437	.0100161	ζ_{13}	.0021562
ζ_{14}	189.18575	.1458893	-.0803417	.0284132	ζ_{14}	.0096970
ζ_{15}	99.098613	.2925544	-.1613876	.0569408	ζ_{15}	.0356721
ζ_{16}	52.351400	.3795955	-.1916860	.0665730	ζ_{16}	.1018044
ζ_{17}	27.812067	.2482997	.0124438	-.0192115	ζ_{17}	.2170369
ζ_{18}	14.828806	.0632815	.3572159	-.1597211	ζ_{18}	.3163362
ζ_{19}	7.9240379	.0060808	.4638703	-.2059025	ζ_{19}	.3210836
ζ_{20}	4.2399181	-.0001173	.2373215	-.0103677	ζ_{20}	.2122959
ζ_{21}	2.2703218	.0003984	.0420742	.2939496	ζ_{21}	.0798722
ζ_{22}	1.2161428	-.0002547	.0042730	.4000842	ζ_{22}	.0199406
ζ_{23}	0.6515723	.0001520	-.0006376	.3137250		
ζ_{24}	.34912095	-.0000740	.0003963	.1296326		
ζ_{25}	.18706936	.0000216	-.0001328	.0381663		

Table 83. Bi ^{4}S (28s, 24p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	24	18	12
Nuclear charge	83	Number of closed shells	6	4	3	1
No. of electrons	83	Open-shell occupation	0	3	0	0

Coupling coefficients

$K_0^{pp} = -0.33333333$ $K_2^{pp} = -0.13333333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-20095.58511	-40191.17440	20095.58930	-1.99999979

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-3000.15226	-512.84150	-125.40472	-29.58729	-5.49767	-0.55165
ζ_1	81466050.	.0000035	-.0000012	.0000006	-.0000003	.0000001	.0000000
ζ_2	16616094.	.0000194	-.0000065	.0000031	-.0000016	.0000007	-.0000002
ζ_3	3918843.6	.0001102	-.0000368	.0000175	-.0000088	.0000039	-.0000013
ζ_4	1057867.4	.0005099	-.0001703	.0000812	-.0000409	.0000183	-.0000060
ζ_5	322990.53	.0020310	-.0006797	.0003240	-.0001632	.0000729	-.0000239
ζ_6	110076.89	.0070118	-.0023581	.0011258	-.0005673	.0002538	-.0000831
ζ_7	41290.502	.0212570	-.0072382	.0034588	-.0017430	.0007790	-.0002550
ζ_8	16805.390	.0565811	-.0198265	.0095289	-.0048098	.0021536	-.0007055
ζ_9	7319.0317	.1299186	-.0484257	.0234611	-.0118616	.0053034	-.0017358
ζ_{10}	3366.9167	.2439005	-.1029670	.0510096	-.0259429	.0116454	-.0038180
ζ_{11}	1617.1036	.3337848	-.1779448	.0913891	-.0468667	.0210023	-.0068740
ζ_{12}	802.81715	.2648392	-.2000524	.1110112	-.0581274	.0263692	-.0086730
ζ_{13}	408.54927	.0819892	.0001163	-.0031483	.0020144	-.0012633	.0004738
ζ_{14}	211.69090	.0046561	.4412383	-.3645200	.2105026	-.0965988	.0317014
ζ_{15}	111.09926	.0003715	.5399529	-.6503601	.4172143	-.2000661	.0665944
ζ_{16}	58.822731	-.0001866	.1700488	-.0067108	-.0078395	.0086785	-.0036530
ζ_{17}	31.328173	.0000309	.0078090	.8664301	-.0034039	.5448477	-.1841944
ζ_{18}	16.748492	-.0000258	.0002431	.4362975	-.5895229	.3571986	-.1269008
ζ_{19}	8.9751627	.0000204	-.0001047	.0438198	.7972335	-.6393800	.2397396
ζ_{20}	4.8163589	-.0000078	-.0002227	.0006516	.7633745	-.0120171	.4080079
ζ_{21}	2.5866598	.0000049	.0001977	.0010073	.0822675	.2301928	-.1262539
ζ_{22}	1.3897663	-.0000037	-.0001430	-.0012014	.0221149	.8732620	-.4935388
ζ_{23}	0.7468497	.0000022	.0001138	.0007957	-.0115066	.4275004	-.4375017
ζ_{24}	.40138756	-.0000015	-.0000782	-.0005921	.0086460	.0224887	.0926426
ζ_{25}	.21572963	.0000010	.0000498	.0003858	-.0055590	.0118296	.4953622
ζ_{26}	.11594728	-.0000005	-.0000277	-.0002140	.0030767	-.0056512	.5268569
ζ_{27}	.06231786	.0000002	.0000117	.0000915	-.0013185	.0026491	.1964612
ζ_{28}	.03349382	-.0000001	-.0000027	-.0000215	.0003100	-.0006138	.0158080

Table 83. Bi ^{4}S (28s, 24p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p	6p
	Energy	-493.44878	-116.13388	-25.43746	-3.99460	-0.32007
ζ_5	322990.53	.0000146	-.0000074	.0000037	-.0000016	.0000004
ζ_6	110076.89	.0000682	-.0000344	.0000171	-.0000072	.0000020
ζ_7	41290.502	.0003635	-.0001849	.0000930	-.0000397	.0000109
ζ_8	16805.390	.0015651	-.0007937	.0003964	-.0001676	.0000459
ζ_9	7319.0317	.0060275	-.0030927	.0015577	-.0006646	.0001823
ζ_{10}	3366.9167	.0203499	-.0105333	.0052904	-.0022419	.0006138
ζ_{11}	1617.1036	.0602519	-.0321465	.0163369	-.0069811	.0019155
ζ_{12}	802.81715	.1493180	-.0830010	.0424198	-.0180519	.0049454
ζ_{13}	408.54927	.2862893	-.1708876	.0894270	-.0384998	.0105774
ζ_{14}	211.69090	.3628548	-.2250558	.1181668	-.0504396	.0138173
ζ_{15}	111.09926	.2329556	-.0499202	.0099907	-.0032722	.0008842
ζ_{16}	58.822731	.0513651	.4003722	-.3237519	.1548830	-.0433112
ζ_{17}	31.328173	.0022203	.5335585	-.4525179	.2123492	-.0589293
ζ_{18}	16.748492	-.0001889	.1848099	.1222973	-.0953439	.0279558
ζ_{19}	8.9751627	.0000645	.0193131	.6468604	-.4665549	.1403797
ζ_{20}	4.8163589	-.0001436	-.0011327	.4015264	-.2922917	.0844644
ζ_{21}	2.5866598	.0001098	.0014185	.0502045	.3790441	-.1449063
ζ_{22}	1.3897663	-.0000734	-.0012097	.0094237	.5759347	-.2295206
ζ_{23}	0.7468497	.0000559	.0008132	-.0041437	.2904956	-.1441242
ζ_{24}	.40138756	-.0000372	-.0005771	.0031715	.0373516	.1162011
ζ_{25}	.21572963	.0000239	.0003718	-.0020863	.0083766	.3594307
ζ_{26}	.11594728	-.0000136	-.0002126	.0011971	-.0025570	.4247175
ζ_{27}	.06231786	.0000061	.0000960	-.0005455	.0013967	.2365005
ζ_{28}	.03349382	-.0000016	-.0000250	.0001432	-.0003885	.0507803

	Orbital	3d	4d	5d		4f
	Energy	-99.05616	-17.81798	-1.47706		-7.40852
ζ_8	16805.390	.0000300	-.0000160	.0000059		
ζ_9	7319.0317	.0001294	-.0000670	.0000239		
ζ_{10}	3366.9167	.0007291	-.0003880	.0001423		
ζ_{11}	1617.1036	.0032620	-.0017147	.0006194	ζ_{11}	.0000725
ζ_{12}	802.81715	.0133606	-.0071570	.0026169	ζ_{12}	.0003245
ζ_{13}	408.54927	.0458624	-.0246846	.0089818	ζ_{13}	.0018060
ζ_{14}	211.69090	.1295387	-.0716825	.0263450	ζ_{14}	.0081447
ζ_{15}	111.09926	.2712009	-.1507156	.0551957	ζ_{15}	.0309207
ζ_{16}	58.822731	.3775770	-.1981844	.0721682	ζ_{16}	.0906829
ζ_{17}	31.328173	.2764282	-.0319169	-.0012815	ζ_{17}	.2019087
ζ_{18}	16.748492	.0819069	.3155704	-.1488161	ζ_{18}	.3088907
ζ_{19}	8.9751627	.0089757	.4738470	-.2213995	ζ_{19}	.3278846
ζ_{20}	4.8163589	-.0000420	.2757964	-.0509172	ζ_{20}	.2283720
ζ_{21}	2.5866598	.0004436	.0557917	.2761374	ζ_{21}	.0895420
ζ_{22}	1.3897663	-.0002776	.0059950	.4139367	ζ_{22}	.0229928
ζ_{23}	0.7468497	.0001655	-.0008705	.3287398		
ζ_{24}	.40138756	-.0000804	.0005252	.1302488		
ζ_{25}	.21572963	.0000236	-.0001820	.0369310		

Table 84. Po ^{3}P (28s, 24p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	24	18	12
Nuclear charge	84	Number of closed shells	6	4	3	1
No. of electrons	84	Open-shell occupation	0	4	0	0

Coupling coefficients

$K_0^{pp} = -0.16666667$ $K_2^{pp} = -0.01666667$

Total energy	Potential energy	Kinetic energy	Virial theorem
-20676.49965	-41352.99900	20676.49940	-2.00000001

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-3075.91309	-527.31975	-129.66673	-31.00244	-5.96201	-0.65822
ζ_1	89054877.	.0000032	-.0000011	.0000005	-.0000003	.0000001	.0000000
ζ_2	18260407.	.0000177	-.0000059	.0000028	-.0000014	.0000006	-.0000002
ζ_3	4321596.7	.0001003	-.0000335	.0000160	-.0000081	.0000037	-.0000013
ζ_4	1168814.9	.0004634	-.0001549	.0000739	-.0000374	.0000169	-.0000058
ζ_5	357103.87	.0018466	-.0006182	.0002951	-.0001491	.0000676	-.0000232
ζ_6	121675.42	.0063859	-.0021475	.0010264	-.0005189	.0002353	-.0000808
ζ_7	45605.777	.0194244	-.0066090	.0031620	-.0015992	.0007248	-.0002489
ζ_8	18542.982	.0520064	-.0181700	.0087379	-.0044237	.0020073	-.0006898
ζ_9	8067.8727	.1206829	-.0446732	.0216514	-.0109855	.0049814	-.0017104
ζ_{10}	3708.6113	.2310701	-.0960609	.0475130	-.0242195	.0110128	-.0037869
ζ_{11}	1780.5116	.3284321	-.1701416	.0871088	-.0448106	.0203742	-.0069963
ζ_{12}	883.96157	.2800028	-.2040212	.1121776	-.0586953	.0269158	-.0092811
ζ_{13}	450.04621	.0989461	-.0372512	.0208385	-.0112484	.0049947	-.0016707
ζ_{14}	233.39149	.0070634	.3934179	-.3152384	.1817748	-.0846885	.0291590
ζ_{15}	122.63561	.0006260	.5616656	-.6494696	.4112135	-.1984462	.0692194
ζ_{16}	65.027826	-.0003763	.2113278	-.1349454	.0948027	-.0452211	.0152362
ζ_{17}	34.692601	.0001859	.0121956	.8269812	-.9245268	.5082968	-.1804222
ζ_{18}	18.582303	-.0001532	.0010818	.5212313	-.7447523	.4480799	-.1656215
ζ_{19}	9.9779478	.0001164	-.0007198	.0590688	.6813642	-.5286466	.2065864
ζ_{20}	5.3657299	-.0000785	.0002173	.0048515	.8514792	-.0942775	.4639604
ζ_{21}	2.8879084	.0000569	-.0001369	-.0017873	.1251266	.0828665	-.0618580
ζ_{22}	1.5550123	-.0000411	.0001008	.0009166	.0215996	.9045921	-.5322436
ζ_{23}	0.8374924	.0000284	-.0000568	-.0007677	-.0099133	.4807684	-.5070384
ζ_{24}	.45109815	-.0000192	.0000372	.0004821	.0077655	.0331358	.0960775
ζ_{25}	.24298423	.0000120	-.0000229	-.0002961	-.0050524	.0107047	.5338531
ζ_{26}	.13088522	-.0000066	.0000122	.0001641	.0027888	-.0046053	.5269892
ζ_{27}	.07050250	.0000028	-.0000051	-.0000679	-.0012012	.0022712	.1817208
ζ_{28}	.03797682	-.0000006	.0000012	.0000159	.0002815	-.0005096	.0140497

Table 84. Po ^{3}P (28s, 24p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p	6p
	Energy	-507.64649	-120.23653	-26.75980	-4.40005	-0.34144
ζ_5	357103.87	.0000128	-.0000065	.0000033	-.0000014	.0000004
ζ_6	121675.42	.0000598	-.0000302	.0000151	-.0000065	.0000019
ζ_7	45605.777	.0003194	-.0001627	.0000821	-.0000357	.0000105
ζ_8	18542.982	.0013804	-.0007008	.0003516	-.0001513	.0000443
ζ_9	8067.8727	.0053364	-.0027407	.0013851	-.0006012	.0001766
ζ_{10}	3708.6113	.0181374	-.0093870	.0047340	-.0020414	.0005980
ζ_{11}	1780.5116	.0542098	-.0288759	.0147176	-.0063971	.0018790
ζ_{12}	883.96157	.1367787	-.0757351	.0388311	-.0168134	.0049291
ζ_{13}	450.04621	.2702729	-.1603386	.0840261	-.0367809	.0108175
ζ_{14}	233.39149	.3622476	-.2258468	.1194002	-.0519418	.0152304
ζ_{15}	122.63561	.2554404	-.0873404	.0340102	-.0141909	.0041786
ζ_{16}	65.027826	.0658532	.3482905	-.2817661	.1370540	-.0410878
ζ_{17}	34.692601	.0033615	.5524755	-.4755195	.2292343	-.0682334
ζ_{18}	18.582303	-.0000037	.2254018	.0327311	-.0465617	.0150290
ζ_{19}	9.9779478	-.0000592	.0258626	.6268173	-.4529236	.1462892
ζ_{20}	5.3657299	-.0000682	-.0001252	.4563251	-.3602353	.1142231
ζ_{21}	2.8879084	.0000537	.0008606	.0695326	.3280149	-.1377007
ζ_{22}	1.5550123	-.0000333	-.0008011	.0106417	.6003319	-.2614282
ζ_{23}	0.8374924	.0000287	.0005114	-.0042181	.3177098	-.1684890
ζ_{24}	.45109815	-.0000188	-.0003723	.0033015	.0428113	.1397070
ζ_{25}	.24298423	.0000122	.0002407	-.0021974	.0088834	.3710826
ζ_{26}	.13088522	-.0000070	-.0001372	.0012531	-.0021164	.4108045
ζ_{27}	.07050250	.0000031	.0000622	-.0005780	.0015644	.2294070
ζ_{28}	.03797682	-.0000008	-.0000161	.0001498	-.0003326	.0552252

	Orbital	3d	4d	5d		4f
	Energy	-102.86241	-18.96124	-1.75521		-8.28055
ζ_8	18542.982	.0000256	-.0000138	.0000053		
ζ_9	8067.8727	.0001103	-.0000572	.0000210		
ζ_{10}	3708.6113	.0006278	-.0003368	.0001280		
ζ_{11}	1780.5116	.0028103	-.0014832	.0005531	ζ_{11}	.0000620
ζ_{12}	883.96157	.0116423	-.0062758	.0023754	ζ_{12}	.0002738
ζ_{13}	450.04621	.0404665	-.0218644	.0082197	ζ_{13}	.0015612
ζ_{14}	233.39149	.1169905	-.0650293	.0247258	ζ_{14}	.0070523
ζ_{15}	122.63561	.2535758	-.1418735	.0537271	ζ_{15}	.0274730
ζ_{16}	65.027826	.3727881	-.2006348	.0759507	ζ_{16}	.0824472
ζ_{17}	34.692601	.2978361	-.0651023	.0131954	ζ_{17}	.1899360
ζ_{18}	18.582303	.0993715	.2789604	-.1385281	ζ_{18}	.3023291
ζ_{19}	9.9779478	.0121490	.4769924	-.2324654	ζ_{19}	.3325541
ζ_{20}	5.3657299	.0001195	.3068595	-.0837601	ζ_{20}	.2408392
ζ_{21}	2.8879084	.0004363	.0689880	.2606550	ζ_{21}	.0973125
ζ_{22}	1.5550123	-.0002642	.0075602	.4265790	ζ_{22}	.0252380
ζ_{23}	0.8374924	.0001569	-.0009666	.3402537		
ζ_{24}	.45109815	-.0000760	.0005805	.1290124		
ζ_{25}	.24298423	.0000224	-.0002096	.0348458		

Table 85. At ^{2}P (28s, 24p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	24	18	12
Nuclear charge	85	Number of closed shells	6	4	3	1
No. of electrons	85	Open-shell occupation	0	5	0	0

Coupling coefficients

$K_0^{pp} = -0.06666667$ $K_2^{pp} = 0.00533333$

Total energy	Potential energy	Kinetic energy	Virial theorem
-21266.88050	-42533.75780	21266.87730	-2.00000015

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-3152.63292	-542.01002	-134.00554	-32.44667	-6.43097	-0.76535
ζ_1	92596223.	.0000031	-.0000010	.0000005	-.0000003	.0000001	.0000000
ζ_2	19516300.	.0000165	-.0000055	.0000026	-.0000013	.0000006	-.0000002
ζ_3	4704109.0	.0000920	-.0000308	.0000147	-.0000075	.0000034	-.0000012
ζ_4	1285396.9	.0004216	-.0001410	.0000674	-.0000342	.0000157	-.0000056
ζ_5	394156.98	.0016807	-.0005629	.0002691	-.0001365	.0000627	-.0000224
ζ_6	134109.53	.0058502	-.0019675	.0009414	-.0004775	.0002194	-.0000783
ζ_7	50020.406	.0179899	-.0061171	.0029302	-.0014869	.0006829	-.0002436
ζ_8	20198.482	.0488362	-.0170264	.0081938	-.0041615	.0019128	-.0006828
ζ_9	8722.0802	.1151692	-.0424327	.0205789	-.0104759	.0048138	-.0017171
ζ_{10}	3980.6634	.2247018	-.0925664	.0457614	-.0233932	.0107729	-.0038481
ζ_{11}	1899.5546	.3270789	-.1668571	.0853440	-.0440355	.0202934	-.0072400
ζ_{12}	938.79870	.2884956	-.2063967	.1130524	-.0592636	.0275012	-.0098493
ζ_{13}	476.62446	.1075766	-.0531614	.0308716	-.0167784	.0077091	-.0027113
ζ_{14}	246.90274	.0084578	.3719896	-.2948550	.1702593	-.0804610	.0287843
ζ_{15}	129.79460	.0007177	.5681926	-.6455802	.4077736	-.1988721	.0720612
ζ_{16}	68.947615	-.0004411	.2302309	-.1884496	.1359915	-.0676066	.0240334
ζ_{17}	36.889980	.0002426	.0151714	.7986435	-.8810580	.4910717	-.1812452
ζ_{18}	19.832924	-.0002020	.0013271	.5605070	-.8125131	.4924434	-.1889709
ζ_{19}	10.695760	.0001542	-.0008968	.0704997	.6097627	-.4697990	.1908226
ζ_{20}	5.7792186	-.0001069	.0003447	.0064412	.8933961	-.1381761	.5025191
ζ_{21}	3.1262002	.0000783	-.0002389	-.0027153	.1542517	-.0050597	-.0191760
ζ_{22}	1.6921404	-.0000569	.0001771	.0016418	.0217382	.9230980	-.5676630
ζ_{23}	0.9162125	.0000397	-.0001100	-.0013256	-.0088759	.5134118	-.5618627
ζ_{24}	.49616004	-.0000268	.0000735	.0008696	.0071731	.0385869	.1113956
ζ_{25}	.26870430	.0000169	-.0000459	-.0005415	-.0047249	.0109295	.5613743
ζ_{26}	.14552478	-.0000092	.0000247	.0003006	.0025915	-.0043166	.5251551
ζ_{27}	.07881373	.0000039	-.0000104	-.0001248	-.0011193	.0022190	.1698291
ζ_{28}	.04268421	-.0000009	.0000024	.0000292	.0002605	-.0004841	.0128543

Table 85. At ^{2}P (28s, 24p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p	6p
	Energy	-522.05562	-124.41552	-28.11078	-4.80979	-0.37984
ζ_5	394156.98	.0000112	-.0000057	.0000029	-.0000013	.0000004
ζ_6	134109.53	.0000529	-.0000267	.0000134	-.0000059	.0000018
ζ_7	50020.406	.0002854	-.0001456	.0000738	-.0000326	.0000101
ζ_8	20198.482	.0012530	-.0006371	.0003210	-.0001405	.0000436
ζ_9	8722.0802	.0049191	-.0025284	.0012824	-.0005656	.0001761
ζ_{10}	3980.6634	.0169754	-.0087926	.0044523	-.0019521	.0006060
ζ_{11}	1899.5546	.0514276	-.0273846	.0140038	-.0061848	.0019255
ζ_{12}	938.79870	.1315401	-.0727766	.0374536	-.0164882	.0051228
ζ_{13}	476.62446	.2638431	-.1562161	.0820983	-.0365125	.0113827
ζ_{14}	246.90274	.3615601	-.2259584	.1200638	-.0531436	.0165162
ζ_{15}	129.79460	.2645245	-.1018237	.0433234	-.0186522	.0058293
ζ_{16}	68.947615	.0727413	.3240373	-.2635331	.1303733	-.0414904
ζ_{17}	36.889980	.0041100	.5563316	-.4819976	.2372266	-.0749288
ζ_{18}	19.832924	.0000676	.2452987	-.0104605	-.0229270	.0082772
ζ_{19}	10.695760	-.0001054	.0303299	.6102182	-.4468479	.1536700
ζ_{20}	5.7792186	-.0000410	.0003275	.4836207	-.3970030	.1347718
ζ_{21}	3.1262002	.0000330	.0006518	.0824879	.2987776	-.1356382
ζ_{22}	1.6921404	-.0000183	-.0006489	.0114373	.6154583	-.2903601
ζ_{23}	0.9162125	.0000188	.0003948	-.0041495	.3315161	-.1864101
ζ_{24}	.49616004	-.0000121	-.0002933	.0032956	.0451689	.1624023
ζ_{25}	.26870430	.0000079	.0001906	-.0022196	.0094749	.3860437
ζ_{26}	.14552478	-.0000046	-.0001078	.0012523	-.0017580	.4035543
ζ_{27}	.07881373	.0000020	.0000492	-.0005845	.0017569	.2162848
ζ_{28}	.04268421	-.0000005	-.0000125	.0001486	-.0002857	.0518833

	Orbital	3d	4d	5d		4f
	Energy	-106.74389	-20.13207	-2.03784		-9.17998
ζ_8	20198.482	.0000225	-.0000122	.0000048		
ζ_9	8722.0802	.0000995	-.0000518	.0000196		
ζ_{10}	3980.6634	.0005743	-.0003100	.0001214		
ζ_{11}	1899.5546	.0026090	-.0013848	.0005320	ζ_{11}	.0000572
ζ_{12}	938.79870	.0109395	-.0059302	.0023130	ζ_{12}	.0002567
ζ_{13}	476.62446	.0384152	-.0208680	.0080830	ζ_{13}	.0014815
ζ_{14}	246.90274	.1121700	-.0626746	.0245577	ζ_{14}	.0067172
ζ_{15}	129.79460	.2462447	-.1386661	.0541243	ζ_{15}	.0263822
ζ_{16}	68.947615	.3691470	-.2011661	.0785969	ζ_{16}	.0797005
ζ_{17}	36.889980	.3056429	-.0786805	.0196403	ζ_{17}	.1853671
ζ_{18}	19.832924	.1079117	.2605849	-.1351356	ζ_{18}	.2991134
ζ_{19}	10.695760	.0140809	.4755295	-.2404126	ζ_{19}	.3335169
ζ_{20}	5.7792186	.0002195	.3213848	-.1009881	ζ_{20}	.2448526
ζ_{21}	3.1262002	.0004323	.0767250	.2546593	ζ_{21}	.0999037
ζ_{22}	1.6921404	-.0002583	.0084945	.4365675	ζ_{22}	.0256370
ζ_{23}	0.9162125	.0001528	-.0009832	.3438553		
ζ_{24}	.49616004	-.0000736	.0005803	.1242531		
ζ_{25}	.26870430	.0000219	-.0002202	.0326241		

Table 86. Rn ^{1}S (28s, 24p, 18d, 12f; 28 ζ)

		Symmetry species	S	P	D	F
		Number of basis functions	28	24	18	12
Nuclear charge	86	Number of closed shells	6	5	3	1
No. of electrons	86	Open-shell occupation	0	0	0	0

Total energy	Potential energy	Kinetic energy	Virial theorem
-21866.77108	-43733.54180	21866.77080	-2.00000001

	Orbital	1s	2s	3s	4s	5s	6s
	Energy	-3230.31250	-556.91297	-138.42174	-33.92062	-6.90574	-0.87397
ζ_1	98695815.	.0000029	-.0000010	.0000005	-.0000002	.0000001	.0000000
ζ_2	21091278.	.0000153	-.0000051	.0000024	-.0000012	.0000006	-.0000002
ζ_3	5132142.2	.0000846	-.0000283	.0000135	-.0000069	.0000032	-.0000012
ζ_4	1410319.4	.0003853	-.0001289	.0000617	-.0000314	.0000146	-.0000054
ζ_5	433531.63	.0015355	-.0005145	.0002462	-.0001253	.0000583	-.0000215
ζ_6	147500.43	.0053590	-.0018025	.0008634	-.0004393	.0002043	-.0000752
ζ_7	54913.915	.0165696	-.0056310	.0027005	-.0013751	.0006395	-.0002354
ζ_8	22109.179	.0453524	-.0157771	.0075977	-.0038705	.0018009	-.0006634
ζ_9	9514.2752	.1082357	-.0396696	.0192497	-.0098316	.0045756	-.0016843
ζ_{10}	4327.2744	.2150079	-.0875816	.0432579	-.0221710	.0103329	-.0038083
ζ_{11}	2058.6291	.3222504	-.1610115	.0821986	-.0425345	.0198569	-.0073113
ζ_{12}	1014.9288	.2988377	-.2078293	.1131595	-.0593800	.0278562	-.0102914
ζ_{13}	514.39844	.1214476	-.0764938	.0452435	-.0246913	.0116314	-.0042544
ζ_{14}	266.22284	.0111708	.3363787	-.2617840	.1511851	-.0724555	.0267527
ζ_{15}	139.92336	.0008705	.5761218	-.6356936	.3990050	-.1962063	.0733253
ζ_{16}	74.361553	-.0005475	.2612236	-.2667165	.1947519	-.0996883	.0369667
ζ_{17}	39.826146	.0003408	.0205558	.7520298	-.8124678	.4585415	-.1747808
ζ_{18}	21.441926	-.0002876	.0017748	.6164420	-.8985898	.5464989	-.2158782
ζ_{19}	11.583686	.0002206	-.0012278	.0877286	.5108767	-.3867039	.1616290
ζ_{20}	6.2713843	-.0001569	.0005992	.0091485	.9414438	-.1798056	.5380356
ζ_{21}	3.3996865	.0001158	-.0004435	-.0042955	.1937862	-.1159136	.0384969
ζ_{22}	1.8442936	-.0000842	.0003303	.0028873	.0212422	.9411914	-.5984321
ζ_{23}	1.0008923	.0000590	-.0002183	-.0022745	-.0068822	.5499918	-.6176392
ζ_{24}	.54328083	-.0000399	.0001473	.0015303	.0059319	.0456413	.1214339
ζ_{25}	.29491399	.0000251	-.0000926	-.0009614	-.0039902	.0106116	.5862177
ζ_{26}	.16009530	-.0000137	.0000502	.0005340	.0021693	-.0036678	.5250765
ζ_{27}	.08690909	.0000057	-.0000210	-.0002224	-.0009455	.0020099	.1595605
ζ_{28}	.04717941	-.0000013	.0000049	.0000518	.0002191	-.0004248	.0112606

Table 86. Rn ^{1}S (28s, 24p, 18d, 12f; 28 ζ) (continued)

	Orbital	2p	3p	4p	5p	6p
	Energy	-536.67686	-128.67143	-29.49106	-5.22513	-0.42798
ζ_5	433531.63	.0000099	-.0000050	.0000026	-.0000012	.0000004
ζ_6	147500.43	.0000467	-.0000237	.0000120	-.0000053	.0000017
ζ_7	54913.915	.0002536	-.0001295	.0000658	-.0000295	.0000096
ζ_8	22109.179	.0011219	-.0005713	.0002891	-.0001286	.0000415
ζ_9	9514.2752	.0044405	-.0022842	.0011623	-.0005208	.0001688
ζ_{10}	4327.2744	.0154811	-.0080228	.0040790	-.0018181	.0005874
ζ_{11}	2058.6291	.0474295	-.0252305	.0129407	-.0058059	.0018816
ζ_{12}	1014.9288	.1232427	-.0680424	.0351387	-.0157245	.0050848
ζ_{13}	514.39844	.2527511	-.1490327	.0784817	-.0354484	.0115039
ζ_{14}	266.22284	.3593081	-.2248452	.1200657	-.0540727	.0174936
ζ_{15}	139.92336	.2790181	-.1234986	.0571936	-.0253664	.0082596
ζ_{16}	74.361553	.0844443	.2868846	-.2350052	.1181864	-.0392210
ζ_{17}	39.826146	.0055016	.5610520	-.4884208	.2454679	-.0808253
ζ_{18}	21.441926	.0001905	.2748998	-.0692313	.0103206	-.0026066
ζ_{19}	11.583686	-.0001864	.0371353	.5861611	-.4337136	.1558777
ζ_{20}	6.2713843	.0000116	.0011584	.5181029	-.4406658	.1575334
ζ_{21}	3.3996865	-.0000080	.0002403	.0999806	.2604093	-.1267507
ζ_{22}	1.8442936	.0000116	-.0003354	.0122772	.6333083	-.3169076
ζ_{23}	1.0008923	-.0000017	.0001591	-.0038787	.3486130	-.2055025
ζ_{24}	.54328083	.0000019	-.0001314	.0031559	.0478448	.1804298
ζ_{25}	.29491399	-.0000009	.0000854	-.0021285	.0089630	.4029199
ζ_{26}	.16009530	.0000005	-.0000487	.0012203	-.0022919	.4003792
ζ_{27}	.08690909	-.0000002	.0000220	-.0005573	.0013778	.2028125
ζ_{28}	.04717941	.0000001	-.0000057	.0001448	-.0003536	.0449889

	Orbital	3d	4d	5d		4f
	Energy	-110.70123	-21.33120	-2.32624		-10.10753
ζ_8	22109.179	.0000195	-.0000106	.0000043		
ζ_9	9514.2752	.0000872	-.0000456	.0000177		
ζ_{10}	4327.2744	.0005088	-.0002763	.0001113		
ζ_{11}	2058.6291	.0023307	-.0012433	.0004904	ζ_{11}	.0000507
ζ_{12}	1014.9288	.0098854	-.0053879	.0021594	ζ_{12}	.0002278
ζ_{13}	514.39844	.0351593	-.0191892	.0076331	ζ_{13}	.0013408
ζ_{14}	266.22284	.1044110	-.0585940	.0235865	ζ_{14}	.0061089
ζ_{15}	139.92336	.2346996	-.1329782	.0533312	ζ_{15}	.0244193
ζ_{16}	74.361553	.3639643	-.2012392	.0809471	ζ_{16}	.0749887
ζ_{17}	39.826146	.3180760	-.0981656	.0292287	ζ_{17}	.1780980
ζ_{18}	21.441926	.1210409	.2348786	-.1275306	ζ_{18}	.2947016
ζ_{19}	11.583686	.0170667	.4736737	-.2475393	ζ_{19}	.3360057
ζ_{20}	6.2713843	.0004093	.3411107	-.1232679	ζ_{20}	.2521292
ζ_{21}	3.3996865	.0004068	.0870932	.2442720	ζ_{21}	.1044863
ζ_{22}	1.8442936	-.0002346	.0097306	.4473031	ζ_{22}	.0266013
ζ_{23}	1.0008923	.0001378	-.0009855	.3496943		
ζ_{24}	.54328083	-.0000659	.0005759	.1214543		
ζ_{25}	.29491399	.0000199	-.0002305	.0310263		