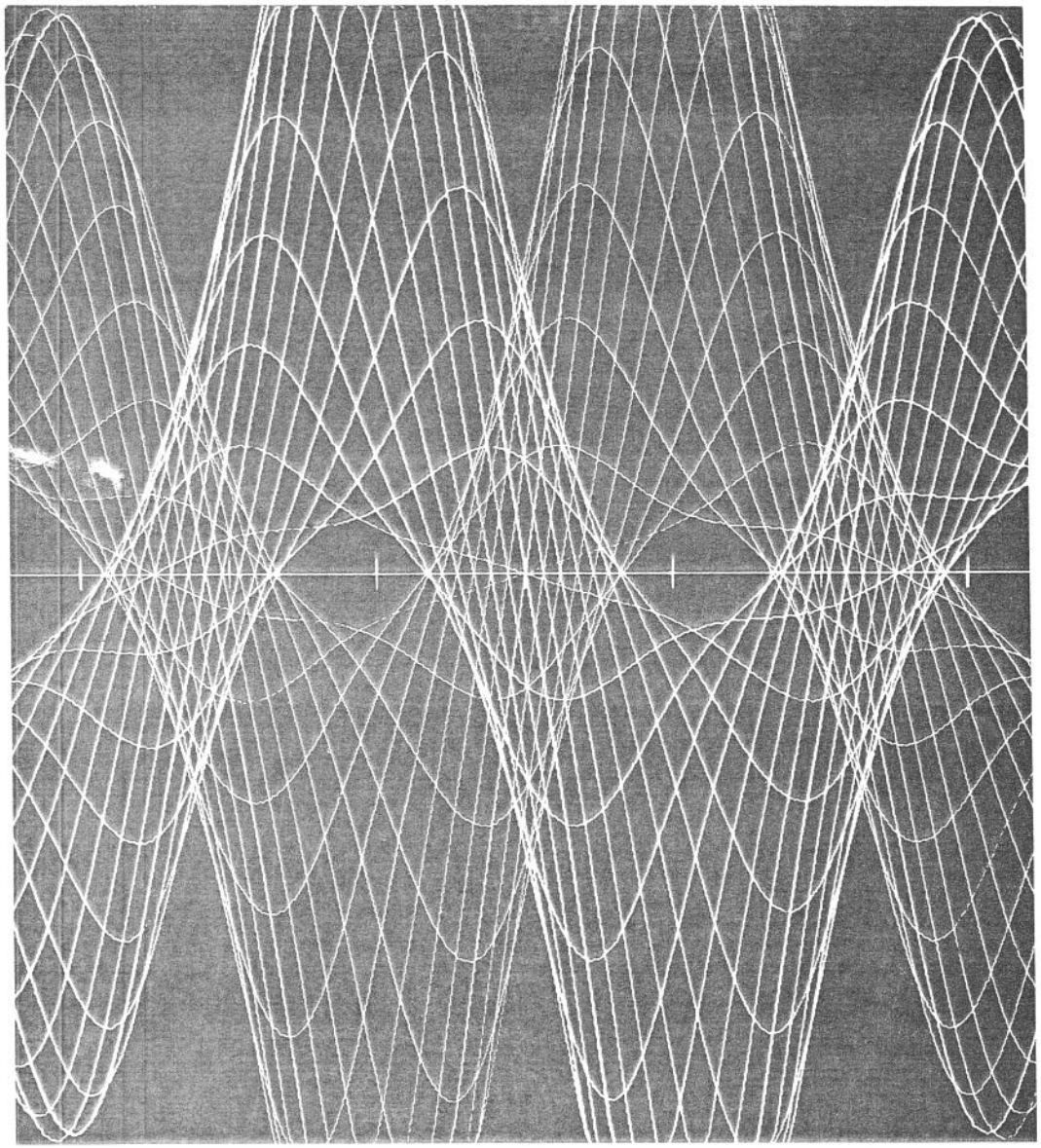

RJ 584

GAUSSIAN BASIS SET FOR MOLECULAR WAVE FUNCTIONS CONTAINING THIRD-ROW ATOMS

A. J.H. Wachters

June 30, 1969

IBM RESEARCH

The cover is designed from an example of an interaction between computers and the physical and mathematical sciences. The design depicts ion trajectories in a type of mass spectrometer used for chemical analysis of residual gases in ultra high vacuum systems. These ion trajectories represent solutions of Mathieu's differential equation. They are generated by numerical integration of the equation using a high speed computer, and are plotted automatically from an output tape as part of the Research Center computing service.

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GAUSSIAN BASIS SET FOR MOLECULAR WAVE FUNCTIONS CONTAINING THIRD-ROW ATOMS

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A Gaussian basis set consisting of 14s-type, 9p-type and 5d type functions has been optimized for the third row atoms up to Zn. Energy values are reported for different contractions of this basis set.

Es wird ein Basissatz von 14s-, 9p- und 5d- Gauß funktionen fur die Atome der dritten Periode bis Zn optimiert. Fur verschiedene Kontraktionen dieser Basis werden die Energiewerten angegeben.

On presente un ensemble optimal de fonctions de base gaussiennes pour les atomes de la troisienne ligne jusqu'a Zn. Cet ensemble comprend 14 fonctions du type s, 9 fonctions du type p et 5 fonctions du type d. On étudie egalement l'effet de differentes contractions de cet ensemble sur l'energie totale.

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To perform ab initio calculation for transition metal - halogenides or - chalcogenides of general geometry one is still resorted to gaussian orbitals for the expansion of the molecular orbitals in the wave function. Since the sets used for these molecules are too large to allow any optimization of the orbital exponents, only optimization of basis set for the atoms can be done in a reasonable computer time. Huzinaga[1] and Veillard[2] optimized basis sets for the first, and second-row atoms respectively. We report here an optimized basis set for the third-row atom up to Zn. Optimization of the basis set was achieved through minimization of the SCF atomic energy with respect to the gaussian orbital exponents. Other methods can also be used such as a least-square fitting of Hartree-Fock orbitals expanded with respect to Slater type orbitals[3,4].

The number of gaussian functions was chosen so that the basis set for the inner shells has the same dimension as the 12s - 9p set reported by Veillard for the second row atoms. By inspection from Veillard's set, this implies that eight 1s functions are used to describe the 1s atomic orbital, two 1s functions for the 2s atomic orbital and two 1s - functions for the 3s atomic orbital, six 2p functions for the 2p atomic orbital and three 2p functions for the 3p atomic orbital. One can expect that the 4s atomic orbital will be adequately represented with two additional 1s functions. As to the 3d atomic orbital, we found that a fair representation could be obtained by using five 3d functions. This makes a total of fourteen 1s functions, nine 2p functions and five 3d functions.

Orbital exponent optimization was performed using the Fortran program ATOM[5]. We first proceeded by optimizing a 12s - 9p basis set for the 18 electron ions K^+, Ca^{2+}, Mn^{7+}, Cu^{11+} and Zn^{12+}. Once this was completed, a fairly good guess could be derived by Lagrange interpolation for the intermediate 18 - electron ions. Starting with these guesses exponent optimization was performed. Then five 3d functions were added to these sets to represent the 3d orbital and optimization of all exponents was performed again for Sc^{2+} to Cu^{2+}, Cu^+ and Zn^{2+}. Finally two 1s functions were added to represent the 4s orbital and optimization of both exponents was performed for the atoms. No reoptimization of the other exponents was performed, as we found that for Zn this gave only a slightly lower energy value (about 0.002 a.u).

Table 1 shows the optimized energy values together with the best results obtained with Slater orbitals. The orbital exponents are reported in Table 2, the orbital energies and expansion coefficients in Table 3. As noticed by Veillard[2], because of the existence of

multiple minima for such a large basis set, it cannot be claimed that the orbital exponents and energy values are fully optimized. However, it seems reasonable that any further optimization would not change more than the last figure given for the total energy. Since these basis sets are intended for molecular calculations, which usually depart from the Hartree-Fock limit by at least 0.01 a.u., this seems of little importance.

For examination of polarisation effects in molecules we also performed optimization of two 2p functions, which were added to the basis set for K^+ to Zn^{2+}, to represent the 4p orbital for the excited configuration $3d^m4p$ of K and Cu(^{2}P) and $3d^m4p^2$ of the other atoms. Table 4 shows the two orbital exponents, the orbital energies and expansion coefficients for the 4p orbital. The orbital energies and expansion coefficients for the other orbitals are given in Table A2 of the Appendix [7]. Table 5a gives the optimized energy values. The radii of maximum charge density R_{max} for 4s- and 4p orbitals are reported in Table 5b. As expected the values of R_{max} for 4p are larger than 4s. For the ground state of atoms with filled 4s and 4p orbitals the radii are almost the same. Therefore the obtained exponents for 4p probable need to be scaled roughly by a factor 1.5. In order to make molecular calculations feasible despite the large number of gaussian functions which are needed, one usually turns to a "contraction", which replaces the individual basis functions whith some appropriate linear combinations. Here the optimized basis set of 14s, 9p and 5d gaussian functions is contracted to 8s-type, 4p-type and 2d-type linear combinations, namely two contracted functions describe each atomic orbital. Given this number of contracted functions, one can think of many different groupings of the basis functions. We concluded from the results obtained by Veillard [2] that the most plausible contractions from energy point of view would be those reported in Table 6. Because contraction of 3d basis functions does not influence the energy value, a (3,2) contraction was chosen, that gives an almost equal splitting of the 3d orbital. The coefficients of the linear combinations are taken equal to the expansion coefficients in Table 3. The corresponding total energies are reported in Table 7 and the lowest value for each atom is also given in Table 1. The normalized contraction coefficients, the orbital energies and expansion coefficients for the three contractions are given in Tables A4, A5 and A6 of the Appendix [7].

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Table 1. Total Energy (in a.u.)

	GTO[a]	CGTO[b]	STO[c]
K(^{2}S)	-599.1559	-599.1429	-599.1645
Ca(^{1}S)	-676.7486	-676.7342	-676.7580
Sc(^{2}D)	-759.7219	-759.7050	-759.7356
Ti(^{3}F)	-848.3890	-848.3685	-848.4052
V(^{4}F)	-942.8620	-942.8372	-942.8829
Cr(^{5}D)	-1043.2818	-1043.2497	-1043.3061
Mn(^{6}S)	-1149.8317	-1149.7872	-1149.8651
Fe(^{5}D)	-1262.4006	-1262.3504	-1262.4425
Co(^{4}F)	-1381.3611	-1381.2895	-1381.4136
Ni(^{3}F)	-1506.8067	-1506.7206	-1506.8690
Cu(^{2}S)	-1638.8735	-1638.8015	-1638.9614
Cu(^{2}D)	-1638.8745	-1638.7867	-1638.9491
Zn(^{1}S)	-1777.7594	-1777.6592	-1777.8470

a. Uncontracted basis set 14s, 9p, 5d.

b. Best result from Table 7.

c. Best result with Slater orbitals from Ref. 6.

TABLE 2. ORBITAL EXPONENTS

	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
1S	150591.	171384.	188961.	206082.	226878.	236658.	243694.	257539.	270991.	284878.	337200.	307637.	316336.
	22629.6	25873.0	28491.4	31226.8	33899.6	35364.0	35995.0	38636.9	39734.8	41997.9	50072.9	46592.9	48561.0
	5223.16	5984.90	6572.43	7199.32	7720.24	8058.31	8223.56	8891.44	9057.46	9627.67	11373.4	10651.1	11157.4
	1498.06	1712.02	1881.03	2048.75	2191.53	2294.23	2353.12	2544.01	2598.21	2761.96	3239.82	3043.31	3205.01
	495.165	563.304	617.979	670.790	719.169	756.118	780.965	844.777	868.200	920.488	1071.97	1010.62	1068.58
	180.792	204.797	225.127	243.650	262.086	277.000	288.519	312.527	323.431	341.805	395.099	374.252	396.394
	71.1940	80.4187	88.5664	95.9250	103.653	110.179	115.701	125.593	130.860	138.023	158.399	150.796	159.806
	29.3723	33.1145	36.5819	39.8101	43.2548	46.3710	49.1175	53.4987	56.1219	59.2587	67.3591	64.6268	68.5890
	8.68863	9.86221	11.0358	12.2205	13.5088	14.8215	16.0885	17.7151	18.9219	20.3712	22.2983	22.1381	23.7081
	3.46382	3.97775	4.49063	5.00882	5.56715	6.13262	6.70430	7.37677	7.95238	8.59400	9.39357	9.34746	10.0372
	.811307	.977055	1.12935	1.28569	1.45174	1.62959	1.80517	2.01847	2.19754	2.39417	2.57848	2.60863	2.81043
	.312555	.396147	.454613	.512806	.574445	.641177	.703011	.779935	.846713	.918169	.964080	.997212	1.06964
	.035668	.065938	.077533	.085576	.092820	.099511	.106385	.114220	.122266	.130176	.113303	.140120	.146951
	.016517	.026902	.030790	.033302	.035532	.037588	.039616	.041889	.044172	.046392	.040791	.049361	.051142
2P	867.259	1000.67	1113.82	1264.70	1398.43	1478.77	1500.39	1678.40	1636.21	1774.18	2245.29	2026.05	2213.18
	205.254	237.310	266.244	301.230	331.571	351.490	358.800	396.392	390.903	423.403	532.106	484.207	527.050
	65.8214	76.4676	86.5763	96.9777	107.002	113.826	116.699	128.598	127.884	138.311	172.195	157.803	172.293
	24.5742	28.7085	32.5934	36.3727	40.3183	43.1567	44.6132	49.1158	49.2413	53.1703	65.3239	60.4844	66.0814
	9.87704	11.6294	13.2190	14.7814	16.4635	17.7775	18.5985	20.5035	20.7512	22.3874	27.0551	25.3593	27.6863
	4.11693	4.90273	5.58357	6.27465	7.02352	7.66128	8.13778	8.98712	9.20368	9.92848	11.7435	11.1685	12.1841
	1.55653	1.92143	2.18594	2.47878	2.79025	3.07765	3.33734	3.68249	3.81779	4.11625	4.69382	4.56411	4.98796
	.614068	.784693	.895011	1.01618	1.14609	1.26619	1.37895	1.52175	1.58762	1.71031	1.90667	1.88440	2.05791
	.228735	.308996	.351975	.398162	.447272	.493534	.538639	.592684	.624660	.672528	.711445	.734735	.798609
3D			22.4283	25.9924	30.2212	34.0221	37.8977	41.4526	44.9774	48.9403	48.5439	53.6478	58.4084
			6.03479	7.08634	8.27218	9.43161	10.5201	11.5403	12.5690	13.7169	13.5490	15.0747	16.4492
			1.97905	2.34871	2.75823	3.15918	3.53764	3.88543	4.24422	4.63951	4.51628	5.10392	5.57570
			.666750	.800198	.942137	1.07995	1.21217	1.32380	1.44330	1.57433	1.47329	1.72743	1.88441
			.218231	.262049	.305298	.346582	.387912	.416680	.449965	.486409	.414875	.528322	.572305

TABLE 3. ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
1S	-133.530	-149.360	-165.890	-183.261	-201.489	-220.576	-240.517	-261.354	-283.044	-305.596	-328.764	-329.008	-353.275
	0.00026	0.00025	0.00025	0.00025	0.00025	0.00027	0.00029	0.00029	0.00031	0.00032	0.00028	0.00031	0.00032
	0.00200	0.00192	0.00193	0.00193	0.00197	0.00208	0.00225	0.00226	0.00242	0.00246	0.00217	0.00236	0.00242
	0.01015	0.00975	0.00980	0.00988	0.01017	0.01071	0.01152	0.01152	0.01238	0.01254	0.01122	0.01213	0.01241
	0.04043	0.03915	0.03940	0.03994	0.04098	0.04284	0.04559	0.04566	0.04849	0.04926	0.04462	0.04791	0.04864
	0.12732	0.12455	0.12532	0.12737	0.12980	0.13420	0.14039	0.14035	0.14672	0.14950	0.13836	0.14652	0.14807
	0.29872	0.29536	0.29577	0.29981	0.30259	0.30798	0.31472	0.31420	0.32127	0.32640	0.31255	0.32298	0.32526
	0.41837	0.41948	0.41900	0.41825	0.41637	0.41361	0.40974	0.40878	0.40497	0.40474	0.41060	0.40665	0.40612
	0.23705	0.24271	0.24139	0.23582	0.23133	0.22241	0.21079	0.21163	0.19961	0.19186	0.21453	0.19742	0.19345
	0.02010	0.02131	0.02141	0.02062	0.02003	0.01895	0.01717	0.01765	0.01561	0.01424	0.01763	0.01507	0.01439
	-0.00372	-0.00413	-0.00418	-0.00393	-0.00370	-0.00337	-0.00285	-0.00292	-0.00242	-0.00202	-0.00296	-0.00222	-0.00206
	0.00114	0.00137	0.00137	0.00126	0.00116	0.00103	0.00084	0.00086	0.00068	0.00055	0.00081	0.00061	0.00055
	-0.00056	-0.00073	-0.00072	-0.00065	-0.00058	-0.00051	-0.00041	-0.00041	-0.00032	-0.00026	-0.00035	-0.00028	-0.00025
	0.00016	0.00022	0.00022	0.00019	0.00016	0.00014	0.00011	0.00011	0.00008	0.00006	0.00008	0.00007	0.00006
	-0.00009	-0.00011	-0.00010	-0.00009	-0.00008	-0.00006	-0.00005	-0.00005	-0.00004	-0.00003	-0.00004	-0.00003	-0.00003
2S	-14.4875	-16.8198	-19.0702	-21.4105	-23.8600	-26.4225	-29.0921	-31.9147	-34.8455	-37.8926	-40.7868	-41.0558	-44.3301
	-0.00008	-0.00007	-0.00007	-0.00008	-0.00008	-0.00008	-0.00009	-0.00009	-0.00009	-0.00010	-0.00008	-0.00009	-0.00010
	-0.00057	-0.00055	-0.00056	-0.00057	-0.00058	-0.00062	-0.00068	-0.00068	-0.00074	-0.00075	-0.00067	-0.00072	-0.00075
	-0.00296	-0.00287	-0.00292	-0.00296	-0.00307	-0.00326	-0.00352	-0.00354	-0.00383	-0.00390	-0.00350	-0.00378	-0.00389
	-0.01178	-0.01153	-0.01172	-0.01199	-0.01241	-0.01308	-0.01404	-0.01415	-0.01513	-0.01545	-0.01400	-0.01508	-0.01538
	-0.04003	-0.03949	-0.04013	-0.04116	-0.04232	-0.04415	-0.04667	-0.04688	-0.04952	-0.05074	-0.04692	-0.04986	-0.05066
	-0.10244	-0.10220	-0.10358	-0.10639	-0.10875	-0.11241	-0.11674	-0.11753	-0.12187	-0.12516	-0.11822	-0.12392	-0.12570
	-0.20507	-0.20618	-0.20845	-0.21157	-0.21369	-0.21630	-0.21957	-0.21962	-0.22348	-0.22667	-0.22445	-0.22696	-0.22907
	-0.13512	-0.14146	-0.14211	-0.13931	-0.13744	-0.13225	-0.12327	-0.12661	-0.11482	-0.10857	-0.12747	-0.11424	-0.11054
	0.50445	0.49875	0.49986	0.50528	0.50776	0.51294	0.52130	0.51771	0.53118	0.53777	0.52939	0.53495	0.54082
	0.61340	0.61749	0.61679	0.61251	0.61106	0.60733	0.59944	0.60469	0.59074	0.58487	0.59487	0.58868	0.58354
	0.05039	0.05569	0.05654	0.05605	0.05604	0.05512	0.05435	0.05456	0.05329	0.05238	0.05316	0.05320	0.05221
	-0.01157	-0.01369	-0.01336	-0.01252	-0.01189	-0.01090	-0.01032	-0.00956	-0.00925	-0.00882	-0.00868	-0.00887	-0.00854
	0.00308	0.00368	0.00359	0.00329	0.00306	0.00271	0.00255	0.00229	0.00220	0.00208	0.00193	0.00207	0.00197
	-0.00177	-0.00176	-0.00166	-0.00152	-0.00141	-0.00125	-0.00117	-0.00106	-0.00101	-0.00095	-0.00093	-0.00094	-0.00089

TABLE 3 (CONTINUED,1).

	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
3S	-1.74718	-2.24362	-2.55908	-2.86328	-3.17094	-3.48486	-3.80139	-4.15079	-4.50330	-4.86422	-4.97894	-5.23343	-5.60783
	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00004	0.00004	0.00003	0.00004	0.00004
	0.00019	0.00019	0.00020	0.00020	0.00021	0.00023	0.00025	0.00025	0.00027	0.00028	0.00025	0.00027	0.00028
	0.00097	0.00099	0.00102	0.00105	0.00111	0.00118	0.00129	0.00131	0.00142	0.00145	0.00130	0.00142	0.00146
	0.00391	0.00400	0.00416	0.00432	0.00452	0.00482	0.00521	0.00529	0.00569	0.00584	0.00529	0.00573	0.00587
	0.01320	0.01364	0.01415	0.01472	0.01531	0.01612	0.01717	0.01738	0.01848	0.01903	0.01756	0.01878	0.01915
	0.03480	0.03633	0.03765	0.03931	0.04072	0.04256	0.04463	0.04527	0.04736	0.04894	0.04609	0.04866	0.04960
	0.07012	0.07391	0.07634	0.07867	0.08043	0.08226	0.08424	0.08505	0.08715	0.08897	0.08774	0.08948	0.09067
	0.05250	0.05752	0.05949	0.05988	0.06033	0.05938	0.05674	0.05857	0.05472	0.05288	0.06042	0.05553	0.05460
	-0.24301	-0.25418	-0.26411	-0.27528	-0.28331	-0.29242	-0.30343	-0.30422	-0.31943	-0.32851	-0.32318	-0.32928	-0.33730
	-0.45125	-0.47814	-0.48635	-0.48855	-0.49094	-0.49110	-0.48683	-0.49503	-0.48419	-0.47968	-0.48160	-0.48257	-0.47716
	0.63176	0.63630	0.64988	0.66091	0.66639	0.66794	0.67644	0.67141	0.68377	0.69074	0.69705	0.69074	0.69909
	0.58733	0.59464	0.58970	0.58548	0.58497	0.58769	0.58337	0.59301	0.58293	0.57828	0.57106	0.57926	0.57224
	0.01483	0.01268	0.01179	0.01130	0.01128	0.01215	0.01120	0.01149	0.01129	0.01104	0.01188	0.01131	0.01085
	-0.00622	-0.00348	-0.00285	-0.00271	-0.00280	-0.00330	-0.00298	-0.00312	-0.00310	-0.00306	-0.00382	-0.00315	-0.00306
4S	-0.14698	-0.19492	-0.20794	-0.21822	-0.22756	-0.23632	-0.24427	-0.25374	-0.26241	-0.27063	-0.22928	-0.27838	-0.28561
	-0.00001	-0.00001	-0.00001	-0.00001	-0.00001	-0.00001	-0.00001	-0.00001	-0.00001	-0.00001	-0.00001	-0.00001	-0.00001
	-0.00004	-0.00005	-0.00005	-0.00005	-0.00005	-0.00005	-0.00005	-0.00005	-0.00006	-0.00006	-0.00004	-0.00006	-0.00006
	-0.00019	-0.00024	-0.00024	-0.00024	-0.00025	-0.00026	-0.00028	-0.00027	-0.00029	-0.00030	-0.00022	-0.00028	-0.00029
	-0.00076	-0.00096	-0.00098	-0.00100	-0.00102	-0.00106	-0.00112	-0.00112	-0.00118	-0.00119	-0.00089	-0.00115	-0.00116
	-0.00253	-0.00323	-0.00332	-0.00338	-0.00343	-0.00353	-0.00367	-0.00366	-0.00382	-0.00387	-0.00294	-0.00375	-0.00376
	-0.00681	-0.00871	-0.00892	-0.00911	-0.00922	-0.00942	-0.00964	-0.00963	-0.00990	-0.01006	-0.00784	-0.00983	-0.00983
	-0.01337	-0.01756	-0.01795	-0.01809	-0.01807	-0.01805	-0.01804	-0.01794	-0.01808	-0.01815	-0.01470	-0.01794	-0.01784
	-0.01081	-0.01421	-0.01454	-0.01433	-0.01412	-0.01362	-0.01275	-0.01294	-0.01192	-0.01135	-0.01081	-0.01170	-0.01130
	0.05066	0.06443	0.06633	0.06771	0.06815	0.06881	0.06976	0.06887	0.07113	0.07191	0.05882	0.07090	0.07126
	0.09076	0.12390	0.12510	0.12308	0.12085	0.11805	0.11411	0.11438	0.11007	0.10720	0.08698	0.10585	0.10276
	-0.14349	-0.20149	-0.20641	-0.20652	-0.20372	-0.19915	-0.19670	-0.19222	-0.19336	-0.19234	-0.15354	-0.18850	-0.18768
	-0.30129	-0.36100	-0.35172	-0.33899	-0.32798	-0.31859	-0.30820	-0.30371	-0.29357	-0.28551	-0.23321	-0.28053	-0.27189
	0.70102	0.63605	0.59618	0.58841	0.58495	0.58361	0.57959	0.57985	0.57688	0.57380	0.45851	0.55598	0.55819
	0.40765	0.52450	0.56369	0.56705	0.56562	0.56176	0.56208	0.55882	0.55968	0.56054	0.64479	0.57619	0.57183

TABLE 3 (CONTINUED,2).

	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
2P	-11.5170	-13.6266	-15.6582	-17.7792	-20.0083	-22.3490	-24.7955	-27.3933	-30.0976	-32.9168	-35.5865	-35.8506	-38.8938
	0.00234	0.00223	0.00223	0.00214	0.00214	0.00228	0.00258	0.00249	0.00296	0.00295	0.00226	0.00267	0.00262
	0.01880	0.01792	0.01764	0.01725	0.01735	0.01836	0.02048	0.02015	0.02336	0.02337	0.01841	0.02133	0.02091
	0.08668	0.08284	0.08123	0.08117	0.08128	0.08503	0.09293	0.09199	0.10343	0.10406	0.08646	0.09690	0.09501
	0.25041	0.24217	0.24040	0.24143	0.24130	0.24761	0.26074	0.25991	0.27954	0.28226	0.25450	0.27103	0.26855
	0.42972	0.42397	0.42517	0.42631	0.42622	0.42718	0.42889	0.42887	0.43268	0.43486	0.43419	0.43492	0.43542
	0.35117	0.35857	0.35972	0.35714	0.35578	0.34579	0.32598	0.32691	0.29861	0.29442	0.33390	0.30995	0.31258
	0.06617	0.07472	0.07423	0.07322	0.07307	0.06934	0.06233	0.06275	0.05128	0.04915	0.06162	0.05399	0.05503
	-0.00438	-0.00389	-0.00396	-0.00342	-0.00313	-0.00254	-0.00159	-0.00161	-0.00095	-0.00081	-0.00195	-0.00126	-0.00110
	0.00152	0.00146	0.00156	0.00150	0.00150	0.00139	0.00116	0.00122	0.00098	0.00096	0.00144	0.00115	0.00116
3P	-0.95317	-1.33935	-1.56731	-1.78613	-2.00831	-2.23605	-2.46582	-2.72536	-2.98717	-3.25614	-3.29411	-3.53202	-3.81186
	-0.00072	-0.00073	-0.00075	-0.00074	-0.00075	-0.00081	-0.00093	-0.00090	-0.00109	-0.00109	-0.00084	-0.00100	-0.00098
	-0.00577	-0.00588	-0.00596	-0.00596	-0.00609	-0.00654	-0.00739	-0.00735	-0.00862	-0.00869	-0.00682	-0.00798	-0.00787
	-0.02738	-0.02793	-0.02825	-0.02886	-0.02943	-0.03127	-0.03466	-0.03472	-0.03958	-0.04018	-0.03327	-0.03765	-0.03713
	-0.08130	-0.08437	-0.08635	-0.08876	-0.09036	-0.09431	-0.10097	-0.10189	-0.11130	-0.11347	-0.10136	-0.10942	-0.10913
	-0.15024	-0.15821	-0.16445	-0.16919	-0.17274	-0.17657	-0.18053	-0.18310	-0.18842	-0.19150	-0.19024	-0.19277	-0.19419
	-0.10923	-0.12362	-0.12493	-0.12441	-0.12391	-0.11758	-0.10431	-0.10420	-0.07949	-0.07385	-0.10132	-0.08468	-0.08651
	0.26387	0.25459	0.27112	0.28086	0.28742	0.30020	0.31650	0.32195	0.35481	0.36598	0.34697	0.36227	0.36108
	0.56842	0.57160	0.57602	0.57709	0.57693	0.57490	0.56935	0.56925	0.55625	0.55273	0.56936	0.55762	0.55852
	0.32743	0.32820	0.30890	0.29986	0.29470	0.28473	0.27354	0.26863	0.24345	0.23441	0.24702	0.23633	0.23768
3D			-0.34224	-0.43611	-0.50160	-0.55859	-0.62657	-0.63090	-0.65653	-0.68496	-0.45950	-0.71439	-0.75355
			0.02140	0.02253	0.02270	0.02328	0.02409	0.02511	0.02627	0.02706	0.03097	0.02727	0.02759
			0.11304	0.11961	0.12248	0.12564	0.13073	0.13626	0.14182	0.14598	0.16196	0.14780	0.14994
			0.31393	0.32700	0.33286	0.33897	0.34648	0.35323	0.35942	0.36418	0.37812	0.36659	0.36929
			0.45818	0.46626	0.46989	0.47139	0.47163	0.46867	0.46613	0.46438	0.45866	0.46395	0.46343
			0.41125	0.38132	0.36970	0.36020	0.34784	0.34395	0.33777	0.33310	0.33574	0.33154	0.32865

TABLE 4. ORBITAL EXPONENTS, ORBITAL ENERGIES AND EXPANSION COEFFICIENTS FOR 4P ORBITAL OF EXCITED STATE.

	K(2P)	CA(3P)	SC(4F)	TI(5G)	V(6G)	CR(7F)	MN(8P)	FE(7F)	CO(6G)	NI(5G)	CU(2S)	CU(2P)	ZN(3P)
2P	.041737	.074979	.089748	.101561	.111248	.120675	.127650	.134915	.141308	.146588	.083141	.155065	.162455
	.015208	.026927	.031032	.034054	.036378	.038610	.040280	.041843	.043402	.044447	.018137	.046199	.047769
4P	-0.09552	-0.14814	-0.15775	-0.16376	-0.16825	-0.17217	-0.17608	-0.17781	-0.18146	-0.18243	-0.04576	-0.18361	-0.18590
	0.00010	0.00015	-0.00015	0.00015	0.00015	0.00015	0.00017	0.00016	0.00018	0.00017	0.00006	0.00015	0.00014
	0.00079	0.00117	-0.00120	0.00119	0.00118	0.00123	0.00134	0.00125	0.00141	0.00133	0.00046	0.00116	0.00109
	0.00379	0.00567	-0.00580	0.00584	0.00580	0.00598	0.00641	0.00602	0.00660	0.00629	0.00232	0.00557	0.00526
	0.01115	0.01687	-0.01748	0.01772	0.01757	0.01779	0.01837	0.01738	0.01824	0.01744	0.00680	0.01588	0.01515
	0.02106	0.03282	-0.03449	0.03497	0.03483	0.03457	0.03425	0.03262	0.03239	0.03092	0.01376	0.02933	0.02830
	0.01426	0.02298	-0.02354	0.02306	0.02226	0.02019	0.01662	0.01539	0.01003	0.00825	0.00517	0.00958	0.00937
	-0.03947	-0.05571	0.06110	-0.06306	-0.06313	-0.06408	-0.06480	-0.06158	-0.06488	-0.06238	-0.02404	-0.05836	-0.05539
	-0.09366	-0.15135	0.15659	-0.15545	-0.15226	-0.14773	-0.14282	-0.13357	-0.12751	-0.11917	-0.05577	-0.11230	-0.10774
	-0.06949	-0.08316	0.07016	-0.05966	-0.05029	-0.04163	-0.03236	-0.02951	-0.01841	-0.01481	-0.00067	-0.01647	-0.01571
	0.46060	0.53864	-0.51980	0.50633	0.49972	0.49161	0.49212	0.48241	0.48367	0.47766	0.37066	0.46358	0.45896
	0.62916	0.57036	-0.59145	0.60481	0.61047	0.61784	0.61579	0.62548	0.62274	0.62853	0.75789	0.64375	0.64899

Table 5a. Total energy (in a.u)

K(^{2}P)	-599.1045
Ca(^{3}P)	-676.5978
Sc(^{4}F)	-759.5628
Ti(^{5}G)	-848.2184
V(^{6}G)	-942.6794
Cr(^{7}F)	-1043.0864
Mn(^{8}P)	-1149.6252
Fe(^{7}F)	-1262.1729
Co(^{6}G)	-1381.1194
Ni(^{5}G)	-1506.5446
Cu(^{2}P)	-1638.7259
Cu(^{4}F)	-1638.5939
Zn(^{3}P)	-1777.4648

Table 5b. Radius of max. charge density (in a.u)

	4s	4p
K	4.30	5.92
Ca	3.47	4.33
Sc	3.25	4.01
Ti	3.08	3.78
V	2.94	3.62
Cr	2.83	3.48
Mn	2.72	3.37
Fe	2.61	3.29
Co	2.52	3.22
Ni	2.43	3.16
Cu	2.62	4.57
Cu	2.35	3.10
Zn	2.28	3.03

TABLE 6. Contraction of the Orbitals.

Contraction No.	Grouping of the Gaussian basis Orbitals.
1.	(1, 2, 3, 4, 5, 6)(7, 8)(9)(10)(11)(12)(13)(14)/(15, 16, 17, 18, 19)(20)(21)(22, 23)/(24, 25, 26)(27, 28)
2.	(1, 2, 3, 4, 5, 6)(7, 8)(9)(10)(11)(12)(13)(14)/(15, 16,17, 18)(19, 20)(21)(22, 23)/(24, 25, 26)(27, 28)
3.	(1, 2, 3, 4, 5, 6)(7, 8)(9)(10)(11)(12)(13)(14)/(15, 16, 17)(18, 19, 20)(21)(22, 23)(24, 25, 26)(27, 28)

Table 7. Total energy (in a.u) from the contracted calculations

	contraction 1	contraction 2	contraction 3
$K(^2S)$	-599.1403	-599.1420	-599.1429
$Ca(^1S)$	-676.7308	-676.7334	-676.7342
$Sc(^2D)$	-759.7007	-759.7036	-759.7050
$Ti(^3F)$	-848.3635	-848.3665	-848.3685
$V(^4F)$	-942.8315	-942.8346	-942.8372
$Cr(^5D)$	-1043.2438	-1043.2461	-1043.2497
$Mn(^6S)$	-1149.7826	-1149.7825	-1149.7872
$Fe(^5D)$	-1262.3462	-1262.3452	-1262.3504
$Co(^4F)$	-1381.2895	-1381.2786	-1381.2829
$Ni(^3F)$	-1506.7206	-1506.7040	-1506.7075
$Cu(^2S)$	-1638.8015	-1638.7931	-1638.7995
$Cu(^2D)$	-1638.7867	-1638.7718	-1638.7767
$Zn(^1S)$	-1777.6592	-1777.6429	-1777.6483

TABLE A1. ORBITAL EXPONENTS

	K(2P)	CA(3P)	SC(4F)	TI(5G)	V(6G)	CR(7F)	MN(8P)	FE(7F)	CO(6G)	NI(5G)	CU(2S)	CU(2P)	ZN(3P)
1S	150591.	171384.	188961.	206082.	226878.	236658.	243694.	257539.	270991.	284878.	337200.	307637.	316336.
	22629.6	25873.0	28491.4	31226.8	33899.6	35364.0	35995.0	38636.9	39734.8	41997.9	50072.9	46592.9	48561.0
	5223.16	5984.90	6572.43	7199.32	7720.24	8058.31	8223.56	8891.44	9057.46	9627.67	11373.4	10651.1	11157.4
	1498.06	1712.02	1881.03	2048.75	2191.53	2294.23	2353.12	2544.01	2598.21	2761.96	3239.82	3043.31	3205.01
	495.165	563.304	617.979	670.790	719.169	756.118	780.965	844.777	868.200	920.488	1071.97	1010.62	1068.58
	180.792	204.797	225.127	243.650	262.086	277.000	288.519	312.527	323.431	341.805	395.099	374.252	396.394
	71.1940	80.4187	88.5664	95.9250	103.653	110.179	115.701	125.593	130.860	138.023	158.399	150.796	159.806
	29.3723	33.1145	36.5819	39.8101	43.2548	46.3710	49.1175	53.4987	56.1219	59.2587	67.3591	64.6268	68.5890
	8.68863	9.86221	11.0358	12.2205	13.5088	14.8215	16.0885	17.7151	18.9219	20.3712	22.2983	22.1381	23.7081
	3.46382	3.97775	4.49063	5.00882	5.56715	6.13262	6.70430	7.37677	7.95238	8.59400	9.39357	9.34746	10.0372
	.811307	.977055	1.12935	1.28569	1.45174	1.62959	1.80517	2.01847	2.19754	2.39417	2.57848	2.60863	2.81043
	.312555	.396147	.454613	.512806	.574445	.641177	.703011	.779935	.846713	.918169	.964080	.997212	1.06964
2P	867.259	1000.67	1113.82	1264.70	1398.43	1478.77	1500.39	1678.40	1636.21	1774.18	2245.29	2026.05	2213.18
	205.254	237.310	266.244	301.230	331.571	351.490	358.800	396.392	390.903	423.403	532.106	484.207	527.050
	65.8214	76.4676	86.5763	96.9777	107.002	113.826	116.699	128.588	127.884	138.311	172.195	157.803	172.293
	24.5742	28.7085	32.5934	36.3727	40.3183	43.1567	44.6132	49.1158	49.2413	53.1703	65.3239	60.4844	66.0814
	9.87704	11.6294	13.2190	14.7814	16.4635	17.7775	18.5985	20.5035	20.7512	22.3874	27.0551	25.3593	27.6863
	4.11683	4.90273	5.58357	6.27465	7.02352	7.66128	8.13778	8.98712	9.20368	9.92848	11.7435	11.1685	12.1841
	1.55653	1.92143	2.18594	2.47878	2.79025	3.07765	3.33734	3.68249	3.81779	4.11625	4.69382	4.56411	4.98796
	.614068	.784693	.895011	1.01618	1.14609	1.26619	1.37895	1.52175	1.58762	1.71031	1.90667	1.88440	2.05791
	.228735	.308996	.351975	.398162	.447272	.493534	.538639	.592684	.624660	.672528	.711445	.734735	.798609
	.041737	.074979	.089748	.101561	.111248	.120675	.127650	.134915	.141308	.146588	.083141	.155065	.162455
	.015208	.026927	.031032	.034054	.036378	.038610	.040280	.041843	.043402	.044447	.018137	.046199	.047769
3D			22.4283	25.9924	30.2212	34.0221	37.8977	41.4526	44.9774	48.9403	48.5439	53.6478	58.4084
			6.03479	7.08634	8.27218	9.43161	10.5201	11.5403	12.5690	13.7169	13.5490	15.0747	16.4492
			1.97905	2.34871	2.75823	3.15918	3.53764	3.88543	4.24422	4.63951	4.51628	5.10392	5.57570
			.666750	.800198	.942137	1.07995	1.21217	1.32380	1.44330	1.57433	1.47329	1.72743	1.88441
			.218231	.262049	.305298	.346582	.387912	.416680	.449965	.486409	.414875	.528322	.572305

TABLE A2. ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	K(2P)	CA(3P)	SC(4F)	TI(5G)	V(6G)	CR(7F)	MN(8P)	FE(7F)	CO(6G)	NI(5G)	CU(2S)	CU(2P)	ZN(3P)
1S	-133.586	-149.455	-165.984	-183.357	-201.589	-220.682	-240.628	-261.476	-283.173	-305.736	-328.902	-329.160	-353.437
	0.00026	0.00025	0.00025	0.00025	0.00025	0.00027	0.00029	0.00029	0.00031	0.00032	0.00028	0.00031	0.00032
	0.00200	0.00192	0.00193	0.00193	0.00197	0.00208	0.00225	0.00226	0.00242	0.00246	0.00217	0.00236	0.00242
	0.01015	0.00975	0.00980	0.00988	0.01017	0.01071	0.01152	0.01152	0.01238	0.01254	0.01122	0.01213	0.01241
	0.04043	0.03915	0.03940	0.03994	0.04098	0.04284	0.04559	0.04566	0.04849	0.04926	0.04462	0.04791	0.04864
	0.12732	0.12455	0.12532	0.12737	0.12980	0.13420	0.14039	0.14035	0.14672	0.14950	0.13836	0.14652	0.14807
	0.29872	0.29536	0.29578	0.29981	0.30259	0.30798	0.31472	0.31420	0.32128	0.32640	0.31255	0.32298	0.32526
	0.41836	0.41945	0.41897	0.41823	0.41635	0.41359	0.40972	0.40876	0.40496	0.40473	0.41059	0.40664	0.40611
	0.23707	0.24274	0.24143	0.23586	0.23136	0.22244	0.21082	0.21165	0.19963	0.19188	0.21454	0.19744	0.19347
	0.02008	0.02126	0.02136	0.02057	0.01999	0.01891	0.01713	0.01761	0.01558	0.01421	0.01761	0.01504	0.01436
	-0.00367	-0.00404	-0.00409	-0.00385	-0.00363	-0.00330	-0.00280	-0.00286	-0.00238	-0.00199	-0.00292	-0.00219	-0.00202
	0.00105	0.00120	0.00120	0.00110	0.00102	0.00092	0.00075	0.00077	0.00061	0.00049	0.00075	0.00055	0.00050
	-0.00045	-0.00052	-0.00051	-0.00046	-0.00042	-0.00038	-0.00030	-0.00031	-0.00025	-0.00020	-0.00029	-0.00022	-0.00020
2S	-14.5425	-16.9128	-19.1620	-21.5047	-23.9580	-26.5251	-29.1997	-32.0322	-34.9695	-38.0279	-40.9208	-41.2020	-44.4850
	-0.00008	-0.00007	-0.00007	-0.00008	-0.00008	-0.00008	-0.00009	-0.00009	-0.00009	-0.00010	-0.00008	-0.00009	-0.00010
	-0.00057	-0.00055	-0.00056	-0.00057	-0.00058	-0.00062	-0.00068	-0.00068	-0.00074	-0.00075	-0.00067	-0.00072	-0.00075
	-0.00296	-0.00287	-0.00292	-0.00296	-0.00307	-0.00326	-0.00352	-0.00354	-0.00383	-0.00390	-0.00350	-0.00378	-0.00389
	-0.01178	-0.01152	-0.01171	-0.01198	-0.01240	-0.01308	-0.01403	-0.01415	-0.01512	-0.01545	-0.01400	-0.01508	-0.01538
	-0.04003	-0.03949	-0.04013	-0.04116	-0.04232	-0.04415	-0.04667	-0.04688	-0.04952	-0.05075	-0.04692	-0.04986	-0.05066
	-0.10242	-0.10216	-0.10354	-0.10635	-0.10871	-0.11237	-0.11670	-0.11749	-0.12184	-0.12512	-0.11819	-0.12388	-0.12567
	-0.20511	-0.20622	-0.20849	-0.21161	-0.21373	-0.21634	-0.21962	-0.21967	-0.22353	-0.22672	-0.22450	-0.22702	-0.22912
	-0.13501	-0.14128	-0.14192	-0.13912	-0.13726	-0.13207	-0.12309	-0.12644	-0.11464	-0.10839	-0.12732	-0.11406	-0.11037
	0.50406	0.49798	0.49907	0.50451	0.50703	0.51226	0.52064	0.51710	0.53056	0.53717	0.52900	0.53437	0.54026
	0.61407	0.61865	0.61799	0.61364	0.61214	0.60832	0.60040	0.60556	0.59161	0.58570	0.59552	0.58951	0.58433
	0.04893	0.05338	0.05422	0.05392	0.05406	0.05337	0.05270	0.05309	0.05185	0.05103	0.05199	0.05185	0.05093
	-0.00957	-0.01040	-0.01008	-0.00952	-0.00913	-0.00849	-0.00808	-0.00757	-0.00733	-0.00702	-0.00718	-0.00708	-0.00685
3S	-1.80042	-2.33154	-2.64627	-2.95307	-3.26492	-3.58378	-3.90553	-4.26579	-4.62527	-4.99820	-5.11453	-5.37886	-5.76225
	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00004	0.00004	0.00003	0.00004	0.00004
	0.00019	0.00019	0.00020	0.00020	0.00021	0.00023	0.00025	0.00025	0.00027	0.00028	0.00025	0.00027	0.00028
	0.00097	0.00099	0.00102	0.00105	0.00111	0.00118	0.00129	0.00130	0.00142	0.00145	0.00130	0.00142	0.00146
	0.00391	0.00400	0.00415	0.00431	0.00452	0.00481	0.00520	0.00528	0.00568	0.00584	0.00529	0.00573	0.00586
	0.01319	0.01361	0.01412	0.01469	0.01528	0.01609	0.01714	0.01735	0.01844	0.01900	0.01754	0.01875	0.01912
	0.03481	0.03629	0.03761	0.03928	0.04068	0.04254	0.04460	0.04524	0.04733	0.04892	0.04610	0.04864	0.04958
	0.07003	0.07371	0.07613	0.07847	0.08023	0.08204	0.08402	0.08482	0.08691	0.08873	0.08758	0.08924	0.09043
	0.05261	0.05757	0.05955	0.05996	0.06043	0.05953	0.05690	0.05874	0.05492	0.05309	0.06063	0.05575	0.05482
	-0.24330	-0.25407	-0.26404	-0.27526	-0.28335	-0.29259	-0.30359	-0.30444	-0.31966	-0.32875	-0.32370	-0.32957	-0.33757
	-0.44997	-0.47590	-0.48401	-0.48622	-0.48856	-0.48855	-0.48438	-0.49243	-0.48159	-0.47709	-0.47951	-0.47995	-0.47466
	0.62607	0.62591	0.63958	0.65106	0.65676	0.65815	0.66730	0.66208	0.67460	0.68173	0.69043	0.68175	0.69056
	0.59671	0.60888	0.60359	0.59867	0.59781	0.60080	0.59546	0.60521	0.59486	0.58991	0.58047	0.59095	0.58331

TABLE A2 (CONTINUED).

	K(2P)	CA(3P)	SC(4F)	TI(5G)	V(6G)	CR(7F)	MN(8P)	FE(7F)	CO(6G)	NI(5G)	CU(2S)	CU(2P)	ZN(3P)
2P	-11.5728	-13.7222	-15.7528	-17.8763	-20.1092	-22.4546	-24.9061	-27.5139	-30.2248	-33.0553	-35.7218	-36.0001	-39.0520
	0.00234	0.00223	0.00223	0.00214	0.00214	0.00228	0.00258	0.00249	0.00296	0.00295	0.00226	0.00267	0.00262
	0.01880	0.01792	0.01764	0.01725	0.01735	0.01836	0.02048	0.02015	0.02336	0.02337	0.01841	0.02133	0.02092
	0.08668	0.08285	0.08124	0.08118	0.08129	0.08504	0.09293	0.09200	0.10344	0.10407	0.08647	0.09691	0.09501
	0.25041	0.24217	0.24040	0.24143	0.24130	0.24761	0.26074	0.25991	0.27955	0.28226	0.25450	0.27103	0.26855
	0.42977	0.42405	0.42525	0.42638	0.42628	0.42723	0.42893	0.42890	0.43270	0.43488	0.43419	0.43494	0.43543
	0.35111	0.35846	0.35960	0.35703	0.35567	0.34569	0.32590	0.32683	0.29855	0.29437	0.33387	0.30989	0.31252
	0.06627	0.07489	0.07443	0.07341	0.07325	0.06950	0.06245	0.06288	0.05137	0.04924	0.06167	0.05409	0.05512
	-0.00465	-0.00436	-0.00447	-0.00388	-0.00356	-0.00291	-0.00187	-0.00186	-0.00113	-0.00095	-0.00200	-0.00142	-0.00125
	0.00185	0.00205	0.00218	0.00206	0.00201	0.00182	0.00146	0.00151	0.00118	0.00113	0.00151	0.00135	0.00135
	-0.00047	-0.00060	-0.00061	-0.00052	-0.00045	-0.00036	-0.00024	-0.00025	-0.00017	-0.00016	-0.00013	-0.00021	-0.00021
	0.00021	0.00024	0.00026	0.00025	0.00026	0.00024	0.00020	0.00017	0.00012	0.00009	0.00004	0.00009	0.00008
3P	-1.00767	-1.43232	-1.66012	-1.88185	-2.10847	-2.34135	-2.57648	-2.84722	-3.11620	-3.39737	-3.43260	-3.68484	-3.97374
	-0.00072	-0.00073	-0.00075	-0.00074	-0.00075	-0.00081	-0.00093	-0.00090	-0.00109	-0.00110	-0.00084	-0.00100	-0.00098
	-0.00577	-0.00589	-0.00597	-0.00596	-0.00610	-0.00654	-0.00739	-0.00735	-0.00862	-0.00869	-0.00682	-0.00798	-0.00787
	-0.02745	-0.02808	-0.02838	-0.02897	-0.02952	-0.03135	-0.03473	-0.03478	-0.03964	-0.04024	-0.03327	-0.03770	-0.03717
	-0.08133	-0.08447	-0.08643	-0.08880	-0.09037	-0.09429	-0.10092	-0.10184	-0.11124	-0.11341	-0.10128	-0.10936	-0.10906
	-0.15084	-0.15941	-0.16549	-0.17011	-0.17355	-0.17730	-0.18120	-0.18370	-0.18898	-0.19200	-0.19035	-0.19321	-0.19460
	-0.10845	-0.12220	-0.12365	-0.12317	-0.12270	-0.11637	-0.10306	-0.10299	-0.07832	-0.07276	-0.10081	-0.08368	-0.08555
	0.26184	0.25100	0.26788	0.27781	0.28446	0.29732	0.31362	0.31911	0.35208	0.36337	0.34552	0.35981	0.35870
	0.57566	0.58496	0.58761	0.58730	0.58599	0.58298	0.57666	0.57601	0.56246	0.55847	0.57154	0.56292	0.56349
	0.31790	0.31209	0.29476	0.28720	0.28333	0.27452	0.26430	0.26036	0.23614	0.22788	0.24477	0.23034	0.23208
	0.00903	0.00863	0.00749	0.00728	0.00732	0.00707	0.00694	0.00646	0.00532	0.00471	0.00445	0.00458	0.00461
	-0.00214	-0.00077	-0.00041	-0.00021	-0.00006	0.00021	0.00046	-0.00003	0.00005	-0.00026	-0.00115	-0.00053	-0.00069
4P	-0.09552	-0.14814	-0.15775	-0.16376	-0.16825	-0.17217	-0.17608	-0.17781	-0.18146	-0.18243	-0.04576	-0.18361	-0.18590
	0.00010	0.00015	0.00015	0.00015	0.00015	0.00015	0.00017	0.00016	0.00018	0.00017	0.00006	0.00015	0.00014
	0.00079	0.00117	0.00120	0.00119	0.00118	0.00123	0.00134	0.00125	0.00141	0.00133	0.00046	0.00116	0.00109
	0.00379	0.00567	0.00580	0.00584	0.00580	0.00598	0.00641	0.00602	0.00660	0.00629	0.00232	0.00557	0.00526
	0.01115	0.01687	0.01748	0.01772	0.01757	0.01778	0.01837	0.01738	0.01824	0.01744	0.00680	0.01588	0.01515
	0.02106	0.03282	0.03449	0.03497	0.03483	0.03457	0.03425	0.03262	0.03239	0.03092	0.01376	0.02933	0.02830
	0.01426	0.02298	0.02354	0.02306	0.02226	0.02019	0.01662	0.01539	0.01003	0.00825	0.00517	0.00958	0.00937
	-0.03947	-0.05571	-0.06110	-0.06306	-0.06313	-0.06408	-0.06480	-0.06158	-0.06488	-0.06238	-0.02404	-0.05836	-0.05539
	-0.09366	-0.15135	-0.15659	-0.15545	-0.15226	-0.14773	-0.14282	-0.13357	-0.12751	-0.11917	-0.05577	-0.11230	-0.10774
	-0.06949	-0.08316	-0.07016	-0.05966	-0.05029	-0.04163	-0.03236	-0.02951	-0.01841	-0.01481	-0.00067	-0.01647	-0.01571
	0.46060	0.53864	0.51980	0.50633	0.49972	0.49161	0.49212	0.48241	0.48367	0.47766	0.37066	0.46358	0.45896
	0.62916	0.57036	0.59145	0.60481	0.61047	0.61785	0.61579	0.62549	0.62274	0.62853	0.75789	0.64375	0.64899
3D			-0.43735	-0.53254	-0.60252	-0.66443	-0.73808	-0.75231	-0.78500	-0.82483	-0.59754	-0.86535	-0.91353
			0.02148	0.02261	0.02278	0.02335	0.02415	0.02519	0.02634	0.02714	0.03103	0.02734	0.02765
			0.11353	0.12004	0.12294	0.12611	0.13119	0.13685	0.14239	0.14658	0.16242	0.14838	0.15048
			0.31527	0.32826	0.33412	0.34009	0.34742	0.35414	0.36015	0.36485	0.37851	0.36717	0.36977
			0.45992	0.46752	0.47153	0.47337	0.47394	0.47193	0.46953	0.46805	0.46165	0.46764	0.46694
			0.40749	0.37811	0.36593	0.35605	0.34335	0.33806	0.33182	0.32678	0.33063	0.32526	0.32272

TABLE A3. ORBITAL EXPONENTS

	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
1S	150591.	171384.	188961.	206082.	226878.	236658.	243694.	257539.	270991.	284878.	337200.	307637.	316336.
	22629.6	25873.0	28491.4	31226.8	33899.6	35364.0	35995.0	38636.9	39734.8	41997.9	50072.9	46592.9	48561.0
	5223.16	5984.90	6572.43	7199.32	7720.24	8058.31	8223.56	8891.44	9057.46	9627.67	11373.4	10651.1	11157.4
	1498.06	1712.02	1881.03	2048.75	2191.53	2294.23	2353.12	2544.01	2598.21	2761.96	3239.82	3043.31	3205.01
	495.165	563.304	617.979	670.790	719.169	756.118	780.965	844.777	868.200	920.488	1071.97	1010.62	1068.58
	180.792	204.797	225.127	243.650	262.086	277.000	288.519	312.527	323.431	341.805	395.099	374.252	396.394
	71.1940	80.4187	88.5664	95.9250	103.653	110.179	115.701	125.593	130.860	138.023	158.399	150.796	159.806
	29.3723	33.1145	36.5819	39.8101	43.2548	46.3710	49.1175	53.4987	56.1219	59.2587	67.3591	64.6268	68.5890
	8.68863	9.86221	11.0358	12.2205	13.5088	14.8215	16.0885	17.7151	18.9219	20.3712	22.2983	22.1381	23.7081
	3.46382	3.97775	4.49063	5.00882	5.56715	6.13262	6.70430	7.37677	7.95238	8.59400	9.39357	9.34746	10.0372
	.811307	.977055	1.12935	1.28569	1.45174	1.62959	1.80517	2.01847	2.19754	2.39417	2.57848	2.60863	2.81043
	.312555	.396147	.454613	.512806	.574445	.641177	.703011	.779935	.846713	.918169	.964080	.997212	1.06964
	.035668	.065938	.077533	.085576	.092820	.099511	.106385	.114220	.122266	.130176	.113303	.140120	.146951
	.016517	.026902	.030790	.033302	.035532	.037588	.039616	.041889	.044172	.046392	.040791	.049361	.051142
2P	867.259	1000.67	1113.82	1264.70	1398.43	1478.77	1500.39	1678.40	1636.21	1774.18	2245.29	2026.05	2213.18
	205.254	237.310	266.244	301.230	331.571	351.490	358.800	396.392	390.903	423.403	532.106	484.207	527.050
	65.8214	76.4676	86.5763	96.9777	107.002	113.826	116.699	128.588	127.884	138.311	172.195	157.803	172.293
	24.5742	28.7085	32.5934	36.3727	40.3183	43.1567	44.6132	49.1158	49.2413	53.1703	65.3239	60.4844	66.0814
	9.87704	11.6294	13.2190	14.7814	16.4635	17.7775	18.5985	20.5035	20.7512	22.3874	27.0551	25.3593	27.6863
	4.11693	4.90273	5.58357	6.27465	7.02352	7.66128	8.13778	8.98712	9.20368	9.92848	11.7435	11.1685	12.1841
	1.55653	1.92143	2.18594	2.47878	2.79025	3.07765	3.33734	3.68249	3.81779	4.11625	4.69382	4.56411	4.98796
	.614068	.784693	.895011	1.01618	1.14609	1.26619	1.37895	1.52175	1.58762	1.71031	1.90667	1.88440	2.05791
	.228735	.308996	.351975	.398162	.447272	.493534	.538639	.592684	.624660	.672528	.711445	.734735	.798609
3D			22.4283	25.9924	30.2212	34.0221	37.8977	41.4526	44.9774	48.9403	48.5439	53.6478	58.4084
			6.03479	7.08634	8.27218	9.43161	10.5201	11.5403	12.5690	13.7169	13.5490	15.0747	16.4492
			1.97905	2.34871	2.75823	3.15918	3.53764	3.88543	4.24422	4.63951	4.51628	5.10392	5.57570
			.666750	.800198	.942137	1.07995	1.21217	1.32380	1.44330	1.57433	1.47329	1.72743	1.88441
			.218231	.262049	.305298	.346582	.387912	.416680	.449965	.486409	.414875	.528322	.572305

TABLE A4.1 CONTRACTION COEFFICIENTS (NORMALIZED)

NC	NB	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
1	1	0.00059	0.00058	0.00058	0.00058	0.00057	0.00058	0.00061	0.00062	0.00063	0.00063	0.00059	0.00063	0.00065
	2	0.00454	0.00443	0.00444	0.00438	0.00440	0.00453	0.00476	0.00478	0.00496	0.00497	0.00464	0.00482	0.00492
	3	0.02306	0.02252	0.02256	0.02241	0.02278	0.02340	0.02438	0.02439	0.02538	0.02530	0.02398	0.02483	0.02519
	4	0.09182	0.09036	0.09067	0.09065	0.09176	0.09360	0.09646	0.09670	0.09942	0.09937	0.09540	0.09811	0.09870
	5	0.28915	0.28748	0.28836	0.28904	0.29065	0.29323	0.29704	0.29723	0.30084	0.30158	0.29585	0.30005	0.30049
	6	0.67840	0.68174	0.68055	0.68034	0.67755	0.67294	0.66589	0.66540	0.65874	0.65843	0.66829	0.66140	0.66008
2	7	0.65883	0.65404	0.65491	0.65971	0.66288	0.67001	0.67965	0.67808	0.68874	0.69724	0.67610	0.69211	0.69619
	8	0.37330	0.37842	0.37730	0.37197	0.36828	0.36029	0.34965	0.35105	0.33947	0.33052	0.35324	0.33601	0.33163
3	9	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
4	10	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
5	11	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
6	12	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
7	13	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
8	14	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
9	15	0.00334	0.00326	0.00326	0.00312	0.00312	0.00327	0.00359	0.00347	0.00396	0.00392	0.00317	0.00363	0.00357
	16	0.02686	0.02616	0.02580	0.02516	0.02530	0.02637	0.02855	0.02813	0.03122	0.03104	0.02590	0.02896	0.02853
	17	0.12383	0.12093	0.11883	0.11842	0.11850	0.12210	0.12951	0.12847	0.13827	0.13820	0.12163	0.13159	0.12959
	18	0.35775	0.35355	0.35168	0.35222	0.35181	0.35557	0.36340	0.36299	0.37368	0.37486	0.35801	0.36804	0.36631
	19	0.61392	0.61896	0.62199	0.62194	0.62140	0.61343	0.59776	0.59896	0.57838	0.57753	0.61079	0.59061	0.59394
10	20	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
11	21	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
12	22	0.67556	0.67218	0.68807	0.69548	0.69960	0.70654	0.71303	0.71713	0.73230	0.73883	0.73799	0.73957	0.73908
	23	0.38914	0.38596	0.36899	0.36138	0.35737	0.34994	0.34257	0.33841	0.32050	0.31333	0.32018	0.31344	0.31451
13	24			0.05381	0.05412	0.05346	0.05369	0.05409	0.05499	0.05617	0.05687	0.06164	0.05684	0.05696
	25			0.28432	0.28731	0.28844	0.28981	0.29357	0.29842	0.30331	0.30676	0.32240	0.30803	0.30959
	26			0.78957	0.78545	0.78388	0.78187	0.77811	0.77360	0.76869	0.76529	0.75267	0.76405	0.76251
14	27			0.58994	0.61520	0.62663	0.63538	0.64499	0.64800	0.65232	0.65591	0.66047	0.65796	0.66068
	28			0.52950	0.50313	0.49302	0.48551	0.47569	0.47556	0.47269	0.47048	0.48347	0.47018	0.46854

NC IS CONTRACTION SEQUENCE NUMBER

NB IS BASIS FUNCTION SEQUENCE NUMBER

TABLE A4.2 ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
1S	-133.529	-149.358	-165.887	-183.259	-201.488	-220.577	-240.521	-261.357	-283.051	-305.605	-328.768	-329.016	-353.286
	0.44032	0.43323	0.43460	0.44067	0.44658	0.45765	0.47262	0.47219	0.48770	0.49572	0.46767	0.48832	0.49275
	0.63502	0.64137	0.63979	0.63399	0.62813	0.61732	0.60287	0.60285	0.58800	0.58051	0.60732	0.58757	0.58335
	0.02011	0.02132	0.02142	0.02062	0.02004	0.01896	0.01717	0.01765	0.01561	0.01423	0.01764	0.01507	0.01439
	-0.00372	-0.00414	-0.00418	-0.00393	-0.00370	-0.00337	-0.00285	-0.00292	-0.00242	-0.00202	-0.00296	-0.00223	-0.00206
	0.00114	0.00138	0.00137	0.00126	0.00116	0.00103	0.00084	0.00086	0.00068	0.00055	0.00081	0.00061	0.00055
	-0.00056	-0.00073	-0.00072	-0.00065	-0.00058	-0.00051	-0.00041	-0.00041	-0.00032	-0.00026	-0.00035	-0.00028	-0.00025
	0.00016	0.00022	0.00022	0.00019	0.00016	0.00014	0.00011	0.00011	0.00008	0.00006	0.00008	0.00007	0.00006
	-0.00009	-0.00011	-0.00010	-0.00009	-0.00008	-0.00006	-0.00005	-0.00005	-0.00004	-0.00003	-0.00004	-0.00003	-0.00003
2S	-14.4825	-16.8146	-19.0643	-21.4033	-23.8512	-26.4111	-29.0766	-31.8979	-34.8226	-37.8647	-40.7658	-41.0283	-44.2981
	-0.13972	-0.13870	-0.14062	-0.14418	-0.14759	-0.15291	-0.15974	-0.16052	-0.16759	-0.17171	-0.16129	-0.16954	-0.17210
	-0.33158	-0.33749	-0.34069	-0.34228	-0.34368	-0.34336	-0.34136	-0.34412	-0.34099	-0.34042	-0.35033	-0.34448	-0.34454
	0.49612	0.48761	0.48898	0.49637	0.50040	0.50873	0.52295	0.51750	0.53923	0.54978	0.53139	0.54399	0.55267
	0.61894	0.62528	0.62440	0.61857	0.61588	0.60967	0.59729	0.60385	0.58367	0.57482	0.59244	0.58084	0.57361
	0.04809	0.05199	0.05296	0.05335	0.05405	0.05447	0.05607	0.05563	0.05756	0.05818	0.05493	0.05784	0.05787
	-0.01038	-0.01161	-0.01138	-0.01105	-0.01083	-0.01056	-0.01118	-0.01008	-0.01131	-0.01158	-0.00948	-0.01107	-0.01120
	0.00270	0.00299	0.00293	0.00282	0.00272	0.00261	0.00280	0.00244	0.00279	0.00284	0.00214	0.00267	0.00268
	-0.00155	-0.00142	-0.00135	-0.00130	-0.00125	-0.00120	-0.00129	-0.00113	-0.00128	-0.00131	-0.00104	-0.00122	-0.00122
3S	-1.74512	-2.24139	-2.55657	-2.86038	-3.16765	-3.48103	-3.79685	-4.14580	-4.49734	-4.85740	-4.97267	-5.22637	-5.60000
	0.04640	0.04821	0.04992	0.05196	0.05382	0.05631	0.05930	0.06005	0.06312	0.06504	0.06095	0.06449	0.06572
	0.11774	0.12564	0.12984	0.13279	0.13524	0.13682	0.13754	0.13985	0.13997	0.14082	0.14428	0.14312	0.14394
	-0.23436	-0.24369	-0.25303	-0.26436	-0.27251	-0.28247	-0.29562	-0.29555	-0.31393	-0.32436	-0.31448	-0.32365	-0.33255
	-0.45795	-0.48654	-0.49528	-0.49734	-0.49957	-0.49895	-0.49280	-0.50168	-0.48817	-0.48249	-0.48827	-0.48661	-0.48043
	0.63472	0.64061	0.65449	0.66534	0.67062	0.67156	0.67871	0.67405	0.68458	0.69070	0.69959	0.69152	0.69933
	0.58591	0.59221	0.58711	0.58308	0.58276	0.58592	0.58246	0.59192	0.58294	0.57881	0.57012	0.57931	0.57262
	0.01560	0.01383	0.01299	0.01241	0.01230	0.01301	0.01179	0.01214	0.01160	0.01122	0.01240	0.01162	0.01108
	-0.00666	-0.00404	-0.00343	-0.00324	-0.00329	-0.00371	-0.00326	-0.00342	-0.00324	-0.00313	-0.00408	-0.00329	-0.00315
4S	-0.14686	-0.19481	-0.20782	-0.21808	-0.22741	-0.23616	-0.24409	-0.25355	-0.26218	-0.27038	-0.22905	-0.27814	-0.28535
	-0.00895	-0.01147	-0.01174	-0.01195	-0.01210	-0.01236	-0.01270	-0.01267	-0.01309	-0.01325	-0.01026	-0.01292	-0.01292
	-0.02298	-0.03019	-0.03087	-0.03089	-0.03074	-0.03040	-0.02983	-0.02987	-0.02939	-0.02907	-0.02460	-0.02904	-0.02866
	0.04827	0.06137	0.06313	0.06460	0.06511	0.06601	0.06746	0.06642	0.06939	0.07048	0.05665	0.06916	0.06974
	0.09249	0.12623	0.12755	0.12547	0.12315	0.12014	0.11572	0.11611	0.11114	0.10800	0.08850	0.10693	0.10365
	-0.14392	-0.20233	-0.20733	-0.20739	-0.20452	-0.19976	-0.19690	-0.19253	-0.19310	-0.19185	-0.15384	-0.18828	-0.18732
	-0.30099	-0.36038	-0.35102	-0.33839	-0.32744	-0.31821	-0.30810	-0.30353	-0.29376	-0.28586	-0.23291	-0.28070	-0.27216
	0.69861	0.63404	0.59414	0.58656	0.58309	0.58181	0.57779	0.57800	0.57501	0.57194	0.45627	0.55415	0.55638
	0.40996	0.52627	0.56544	0.56865	0.56724	0.56337	0.56374	0.56051	0.56144	0.56233	0.64680	0.57790	0.57355

TABLE A4.2 (CONTINUED).

	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
2P	-11.5176	-13.6274	-15.6593	-17.7804	-20.0096	-22.3507	-24.7976	-27.3954	-30.1004	-32.9203	-35.5895	-35.8542	-38.8979
	0.69981	0.68482	0.68342	0.68532	0.68577	0.69627	0.71743	0.71595	0.74804	0.75295	0.71078	0.73635	0.73307
	0.35205	0.35941	0.36058	0.35793	0.35653	0.34645	0.32647	0.32743	0.29898	0.29476	0.33449	0.31038	0.31299
	0.06386	0.07254	0.07200	0.07119	0.07111	0.06762	0.06103	0.06141	0.05029	0.04822	0.06006	0.05281	0.05388
	-0.00163	-0.00125	-0.00121	-0.00086	-0.00062	-0.00029	0.00018	0.00025	0.00048	0.00056	0.00021	0.00043	0.00057
3P	-0.95166	-1.33774	-1.56544	-1.78395	-2.00582	-2.23319	-2.46256	-2.72171	-2.98295	-3.25154	-3.28906	-3.52699	-3.80653
	-0.23172	-0.24268	-0.25026	-0.25700	-0.26212	-0.27058	-0.28285	-0.28598	-0.30295	-0.30800	-0.29018	-0.30338	-0.30407
	-0.11958	-0.13442	-0.13670	-0.13699	-0.13720	-0.13199	-0.12030	-0.12063	-0.09819	-0.09312	-0.11867	-0.10344	-0.10526
	0.27094	0.26219	0.27939	0.28972	0.29679	0.31037	0.32787	0.33360	0.36816	0.37975	0.35905	0.37554	0.37435
	0.83885	0.84762	0.83413	0.82653	0.82124	0.80998	0.79439	0.78959	0.75475	0.74311	0.76709	0.74912	0.75086
3D			-0.34133	-0.43503	-0.50040	-0.55727	-0.62513	-0.62938	-0.65498	-0.68340	-0.45772	-0.71271	-0.75182
			0.39742	0.41620	0.42454	0.43347	0.44523	0.45656	0.46756	0.47587	0.50233	0.47980	0.48431
			0.77679	0.75799	0.74994	0.74197	0.73127	0.72329	0.71459	0.70800	0.69448	0.70513	0.70144

TABLE A5.1 CONTRACTION COEFFICIENTS (NORMALIZED)

NC	NB	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
1	1	0.00059	0.00058	0.00058	0.00058	0.00057	0.00058	0.00061	0.00062	0.00063	0.00063	0.00059	0.00063	0.00065
	2	0.00454	0.00443	0.00444	0.00438	0.00440	0.00453	0.00476	0.00478	0.00496	0.00497	0.00464	0.00482	0.00492
	3	0.02306	0.02252	0.02256	0.02241	0.02278	0.02340	0.02438	0.02439	0.02538	0.02530	0.02398	0.02483	0.02519
	4	0.09182	0.09036	0.09067	0.09065	0.09176	0.09360	0.09646	0.09670	0.09942	0.09937	0.09540	0.09811	0.09870
	5	0.28915	0.28748	0.28836	0.28904	0.29065	0.29323	0.29704	0.29723	0.30084	0.30158	0.29585	0.30005	0.30049
	6	0.67840	0.68174	0.68055	0.68034	0.67755	0.67294	0.66589	0.66540	0.65874	0.65843	0.66829	0.66140	0.66008
2	7	0.65883	0.65404	0.65491	0.65971	0.66288	0.67001	0.67965	0.67808	0.68874	0.69724	0.67610	0.69211	0.69619
	8	0.37330	0.37842	0.37730	0.37197	0.36828	0.36029	0.34965	0.35105	0.33947	0.33052	0.35324	0.33601	0.33163
3	9	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
4	10	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
5	11	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
6	12	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
7	13	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
8	14	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
9	15	0.00711	0.00703	0.00710	0.00679	0.00679	0.00700	0.00744	0.00722	0.00789	0.00780	0.00677	0.00742	0.00735
	16	0.05714	0.05645	0.05612	0.05478	0.05508	0.05647	0.05915	0.05849	0.06217	0.06171	0.05525	0.05918	0.05873
	17	0.26346	0.26099	0.25846	0.25781	0.25800	0.26149	0.26835	0.26708	0.27536	0.27473	0.25950	0.26891	0.26680
	18	0.76112	0.76301	0.76494	0.76679	0.76597	0.76146	0.75297	0.75464	0.74418	0.74520	0.76383	0.75215	0.75416
10	19	0.58087	0.57126	0.57105	0.57328	0.57389	0.58117	0.59626	0.59542	0.61956	0.62430	0.59380	0.61204	0.61026
	20	0.47469	0.48314	0.48313	0.48026	0.47905	0.47043	0.45319	0.45386	0.42759	0.42268	0.45664	0.43617	0.43810
11	21	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
12	22	0.67556	0.67218	0.68807	0.69548	0.69960	0.70654	0.71303	0.71713	0.73230	0.73883	0.73799	0.73957	0.73908
	23	0.38914	0.38596	0.36899	0.36138	0.35737	0.34994	0.34257	0.33841	0.32050	0.31333	0.32018	0.31344	0.31451
13	24			0.05381	0.05412	0.05346	0.05369	0.05409	0.05499	0.05617	0.05687	0.06164	0.05684	0.05696
	25			0.28432	0.28731	0.28844	0.28981	0.29357	0.29842	0.30331	0.30676	0.32240	0.30803	0.30959
	26			0.78957	0.78545	0.78388	0.78187	0.77811	0.77360	0.76869	0.76529	0.75267	0.76405	0.76251
14	27			0.58994	0.61520	0.62663	0.63538	0.64499	0.64800	0.65232	0.65591	0.66047	0.65796	0.66068
	28			0.52950	0.50313	0.49302	0.48551	0.47569	0.47556	0.47269	0.47048	0.48347	0.47018	0.46854

NC IS CONTRACTION SEQUENCE NUMBER

NB IS BASIS FUNCTION SEQUENCE NUMBER

TABLE A5.2 ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
1S	-133.535	-149.364	-165.895	-183.269	-201.500	-220.593	-240.541	-261.379	-283.083	-305.643	-328.803	-329.055	-353.327
	0.44033	0.43324	0.43461	0.44068	0.44659	0.45766	0.47263	0.47220	0.48772	0.49573	0.46768	0.48833	0.49276
	0.63502	0.64137	0.63979	0.63399	0.62813	0.61732	0.60287	0.60285	0.58800	0.58051	0.60732	0.58757	0.58335
	0.02009	0.02130	0.02140	0.02060	0.02002	0.01893	0.01714	0.01762	0.01558	0.01420	0.01760	0.01503	0.01435
	-0.00371	-0.00413	-0.00417	-0.00392	-0.00369	-0.00335	-0.00283	-0.00290	-0.00240	-0.00200	-0.00294	-0.00220	-0.00203
	0.00114	0.00137	0.00137	0.00125	0.00115	0.00103	0.00083	0.00085	0.00067	0.00054	0.00080	0.00060	0.00054
	-0.00056	-0.00073	-0.00072	-0.00064	-0.00058	-0.00050	-0.00040	-0.00040	-0.00032	-0.00026	-0.00035	-0.00028	-0.00025
	0.00016	0.00022	0.00022	0.00019	0.00016	0.00014	0.00011	0.00010	0.00008	0.00006	0.00009	0.00007	0.00006
	-0.00009	-0.00011	-0.00010	-0.00009	-0.00008	-0.00006	-0.00005	-0.00005	-0.00004	-0.00003	-0.00004	-0.00003	-0.00003
2S	-14.4825	-16.8146	-19.0646	-21.4040	-23.8523	-26.4130	-29.0799	-31.9019	-34.8307	-37.8749	-40.7742	-41.0381	-44.3083
	-0.13973	-0.13871	-0.14063	-0.14420	-0.14760	-0.15293	-0.15977	-0.16055	-0.16763	-0.17175	-0.16132	-0.16958	-0.17213
	-0.33161	-0.33751	-0.34071	-0.34232	-0.34371	-0.34340	-0.34142	-0.34417	-0.34107	-0.34050	-0.35041	-0.34456	-0.34462
	0.49629	0.48775	0.48915	0.49657	0.50063	0.50900	0.52328	0.51783	0.53969	0.55028	0.53180	0.54445	0.55313
	0.61881	0.62516	0.62426	0.61841	0.61571	0.60947	0.59706	0.60362	0.58336	0.57448	0.59216	0.58053	0.57329
	0.04806	0.05198	0.05295	0.05333	0.05401	0.05443	0.05601	0.05556	0.05744	0.05805	0.05484	0.05773	0.05777
	-0.01038	-0.01162	-0.01138	-0.01106	-0.01083	-0.01056	-0.01117	-0.01008	-0.01130	-0.01157	-0.00947	-0.01106	-0.01119
	0.00270	0.00299	0.00293	0.00282	0.00272	0.00261	0.00280	0.00244	0.00278	0.00283	0.00213	0.00267	0.00267
	-0.00155	-0.00142	-0.00135	-0.00130	-0.00125	-0.00120	-0.00129	-0.00113	-0.00128	-0.00130	-0.00103	-0.00122	-0.00122
3S	-1.74460	-2.24129	-2.55619	-2.85981	-3.16688	-3.47988	-3.79511	-4.14389	-4.49432	-4.85396	-4.97039	-5.22311	-5.59659
	0.04640	0.04821	0.04991	0.05195	0.05381	0.05630	0.05929	0.06004	0.06311	0.06503	0.06095	0.06448	0.06571
	0.11773	0.12564	0.12984	0.13279	0.13524	0.13681	0.13752	0.13984	0.13995	0.14079	0.14427	0.14310	0.14392
	-0.23438	-0.24375	-0.25308	-0.26441	-0.27257	-0.28253	-0.29567	-0.29560	-0.31397	-0.32441	-0.31457	-0.32371	-0.33262
	-0.45787	-0.48646	-0.49519	-0.49725	-0.49949	-0.49887	-0.49274	-0.50162	-0.48815	-0.48249	-0.48823	-0.48659	-0.48040
	0.63471	0.64065	0.65456	0.66544	0.67075	0.67176	0.67900	0.67438	0.68513	0.69132	0.70011	0.69209	0.69988
	0.58589	0.59215	0.58703	0.58297	0.58263	0.58574	0.58220	0.59163	0.58249	0.57830	0.56969	0.57884	0.57216
	0.01564	0.01385	0.01301	0.01244	0.01233	0.01305	0.01183	0.01217	0.01162	0.01124	0.01243	0.01165	0.01110
	-0.00668	-0.00405	-0.00344	-0.00325	-0.00331	-0.00373	-0.00327	-0.00344	-0.00325	-0.00314	-0.00409	-0.00330	-0.00317
4S	-0.14684	-0.19481	-0.20780	-0.21806	-0.22738	-0.23611	-0.24401	-0.25346	-0.26203	-0.27020	-0.22896	-0.27799	-0.28520
	-0.00894	-0.01146	-0.01174	-0.01195	-0.01209	-0.01235	-0.01269	-0.01265	-0.01306	-0.01323	-0.01024	-0.01290	-0.01290
	-0.02297	-0.03019	-0.03086	-0.03088	-0.03072	-0.03037	-0.02979	-0.02983	-0.02934	-0.02901	-0.02457	-0.02899	-0.02862
	0.04825	0.06137	0.06313	0.06459	0.06510	0.06598	0.06742	0.06638	0.06931	0.07039	0.05660	0.06909	0.06967
	0.09240	0.12620	0.12748	0.12537	0.12304	0.11998	0.11550	0.11589	0.11079	0.10762	0.08829	0.10661	0.10335
	-0.14370	-0.20229	-0.20719	-0.20718	-0.20427	-0.19942	-0.19642	-0.19206	-0.19234	-0.19103	-0.15343	-0.18760	-0.18667
	-0.30109	-0.36039	-0.35108	-0.33848	-0.32753	-0.31833	-0.30826	-0.30368	-0.29398	-0.28609	-0.23298	-0.28088	-0.27234
	0.69808	0.63400	0.59396	0.58630	0.58277	0.58136	0.57712	0.57733	0.57390	0.57073	0.45549	0.55314	0.55544
	0.41049	0.52630	0.56562	0.56891	0.56755	0.56381	0.56439	0.56116	0.56253	0.56350	0.64753	0.57887	0.57446

TABLE A5.2 (CONTINUED).

	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
2P	-11.5180	-13.6278	-15.6600	-17.7817	-20.0115	-22.3536	-24.8023	-27.4010	-30.1109	-32.9334	-35.6005	-35.8670	-38.9113
	0.32901	0.31738	0.31427	0.31487	0.31505	0.32522	0.34636	0.34449	0.37576	0.37891	0.33327	0.36046	0.35621
	0.74022	0.74256	0.74497	0.74402	0.74305	0.73537	0.71956	0.72055	0.69855	0.69674	0.73151	0.71084	0.71372
	0.06427	0.07297	0.07241	0.07155	0.07144	0.06787	0.06116	0.06154	0.05028	0.04818	0.06020	0.05284	0.05390
	-0.00179	-0.00141	-0.00137	-0.00100	-0.00075	-0.00040	0.00011	0.00017	0.00044	0.00054	0.00012	0.00038	0.00052
3P	-0.95136	-1.33798	-1.56543	-1.78373	-2.00538	-2.23217	-2.46044	-2.71921	-2.97741	-3.24448	-3.28464	-3.52036	-3.79948
	-0.10587	-0.10921	-0.11170	-0.11462	-0.11691	-0.12284	-0.13301	-0.13405	-0.14873	-0.15157	-0.13247	-0.14500	-0.14425
	-0.25082	-0.27162	-0.28001	-0.28521	-0.28921	-0.28898	-0.28367	-0.28678	-0.27464	-0.27411	-0.29278	-0.28347	-0.28657
	0.27237	0.26151	0.28038	0.29205	0.30039	0.31637	0.33780	0.34465	0.38782	0.40243	0.37464	0.39584	0.39470
	0.83796	0.84753	0.83334	0.82516	0.81934	0.80708	0.78988	0.78462	0.74627	0.73339	0.76022	0.74033	0.74207
3D			-0.34067	-0.43404	-0.49907	-0.55535	-0.62234	-0.62630	-0.65034	-0.67810	-0.45375	-0.70752	-0.74637
			0.39711	0.41587	0.42422	0.43312	0.44487	0.45622	0.46725	0.47561	0.50200	0.47956	0.48408
			0.77702	0.75825	0.75020	0.74224	0.73156	0.72357	0.71485	0.70822	0.69477	0.70533	0.70164

TABLE A6.1 CONTRACTION COEFFICIENTS (NORMALIZED)

NC	NB	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
1	1	0.00059	0.00058	0.00058	0.00058	0.00057	0.00058	0.00061	0.00062	0.00063	0.00063	0.00059	0.00063	0.00065
	2	0.00454	0.00443	0.00444	0.00438	0.00440	0.00453	0.00476	0.00478	0.00496	0.00497	0.00464	0.00482	0.00492
	3	0.02306	0.02252	0.02256	0.02241	0.02278	0.02340	0.02438	0.02439	0.02538	0.02530	0.02398	0.02483	0.02519
	4	0.09182	0.09036	0.09067	0.09065	0.09176	0.09360	0.09646	0.09670	0.09942	0.09937	0.09540	0.09811	0.09870
	5	0.28915	0.28748	0.28836	0.28904	0.29065	0.29323	0.29704	0.29723	0.30084	0.30158	0.29585	0.30005	0.30049
	6	0.67840	0.68174	0.68055	0.68034	0.67755	0.67294	0.66589	0.66540	0.65874	0.65843	0.66829	0.66140	0.66008
2	7	0.65883	0.65404	0.65491	0.65971	0.66288	0.67001	0.67965	0.67808	0.68874	0.69724	0.67610	0.69211	0.69619
	8	0.37330	0.37842	0.37730	0.37197	0.36828	0.36029	0.34965	0.35105	0.33947	0.33052	0.35324	0.33601	0.33163
3	9	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
4	10	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
5	11	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
6	12	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
7	13	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
8	14	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
9	15	0.02316	0.02309	0.02352	0.02266	0.02261	0.02297	0.02370	0.02312	0.02439	0.02418	0.02242	0.02358	0.02352
	16	0.18601	0.18549	0.18594	0.18274	0.18345	0.18518	0.18834	0.18738	0.19210	0.19128	0.18299	0.18807	0.18807
	17	0.85756	0.85762	0.85641	0.85996	0.85927	0.85752	0.85443	0.85563	0.85077	0.85162	0.85949	0.85453	0.85434
10	18	0.27164	0.26383	0.26159	0.26261	0.26261	0.26977	0.28481	0.28378	0.30603	0.30875	0.27628	0.29550	0.29261
	19	0.46615	0.46188	0.46265	0.46371	0.46385	0.46540	0.46848	0.46826	0.47368	0.47568	0.47135	0.47419	0.47444
	20	0.38094	0.39063	0.39142	0.38847	0.38719	0.37672	0.35607	0.35693	0.32691	0.32206	0.36248	0.33794	0.34059
11	21	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
12	22	0.67556	0.67218	0.68807	0.69548	0.69960	0.70654	0.71303	0.71713	0.73230	0.73883	0.73799	0.73957	0.73908
	23	0.38914	0.38596	0.36899	0.36138	0.35737	0.34994	0.34257	0.33841	0.32050	0.31333	0.32018	0.31344	0.31451
13	24			0.05381	0.05412	0.05346	0.05369	0.05409	0.05499	0.05617	0.05687	0.06164	0.05684	0.05696
	25			0.28432	0.28731	0.28844	0.28981	0.29357	0.29842	0.30331	0.30676	0.32240	0.30803	0.30959
	26			0.78957	0.78545	0.78388	0.78187	0.77811	0.77360	0.76869	0.76529	0.75267	0.76405	0.76251
14	27			0.58994	0.61520	0.62663	0.63538	0.64499	0.64800	0.65232	0.65591	0.66047	0.65796	0.66068
	28			0.52950	0.50313	0.49302	0.48551	0.47569	0.47556	0.47269	0.47048	0.48347	0.47018	0.46854

NC IS CONTRACTION SEQUENCE NUMBER

NB IS BASIS FUNCTION SEQUENCE NUMBER

TABLE A6.2 ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
1S	-133.531	-149.359	-165.890	-183.265	-201.497	-220.592	-240.545	-261.385	-283.102	-305.668	-328.816	-329.076	-353.349
	0.44033	0.43324	0.43461	0.44068	0.44659	0.45766	0.47263	0.47221	0.48773	0.49574	0.46769	0.48834	0.49277
	0.63502	0.64137	0.63978	0.63399	0.62812	0.61732	0.60287	0.60284	0.58800	0.58050	0.60732	0.58757	0.58335
	0.02010	0.02131	0.02141	0.02061	0.02002	0.01893	0.01713	0.01761	0.01555	0.01417	0.01759	0.01501	0.01433
	-0.00371	-0.00413	-0.00417	-0.00392	-0.00369	-0.00335	-0.00283	-0.00289	-0.00238	-0.00198	-0.00293	-0.00219	-0.00202
	0.00114	0.00137	0.00137	0.00126	0.00115	0.00103	0.00083	0.00085	0.00067	0.00053	0.00080	0.00059	0.00053
	-0.00056	-0.00073	-0.00072	-0.00065	-0.00058	-0.00050	-0.00040	-0.00040	-0.00032	-0.00025	-0.00035	-0.00027	-0.00025
	0.00016	0.00022	0.00022	0.00019	0.00016	0.00014	0.00011	0.00010	0.00008	0.00006	0.00008	0.00007	0.00006
	-0.00009	-0.00011	-0.00010	-0.00009	-0.00008	-0.00006	-0.00005	-0.00005	-0.00004	-0.00003	-0.00004	-0.00003	-0.00003
2S	-14.4814	-16.8135	-19.0631	-21.4023	-23.8506	-26.4115	-29.0793	-31.9015	-34.8335	-37.8793	-40.7754	-41.0415	-44.3118
	-0.13973	-0.13870	-0.14062	-0.14419	-0.14760	-0.15293	-0.15977	-0.16055	-0.16765	-0.17177	-0.16133	-0.16960	-0.17215
	-0.33158	-0.33748	-0.34068	-0.34229	-0.34369	-0.34339	-0.34141	-0.34417	-0.34110	-0.34054	-0.35042	-0.34458	-0.34464
	0.49617	0.48758	0.48901	0.49645	0.50053	0.50895	0.52331	0.51788	0.53989	0.55052	0.53190	0.54464	0.55331
	0.61889	0.62527	0.62435	0.61849	0.61577	0.60950	0.59703	0.60358	0.58321	0.57430	0.59208	0.58038	0.57314
	0.04811	0.05204	0.05300	0.05337	0.05405	0.05446	0.05602	0.05557	0.05742	0.05801	0.05483	0.05771	0.05775
	-0.01040	-0.01164	-0.01140	-0.01107	-0.01084	-0.01057	-0.01118	-0.01008	-0.01130	-0.01157	-0.00948	-0.01107	-0.01119
	0.00270	0.00300	0.00294	0.00283	0.00273	0.00261	0.00280	0.00244	0.00278	0.00283	0.00213	0.00267	0.00267
	-0.00155	-0.00142	-0.00135	-0.00130	-0.00125	-0.00121	-0.00129	-0.00113	-0.00128	-0.00130	-0.00103	-0.00122	-0.00122
3S	-1.74502	-2.24193	-2.55665	-2.86017	-3.16716	-3.48001	-3.79504	-4.14379	-4.49399	-4.85361	-4.97028	-5.22280	-5.59628
	0.04640	0.04821	0.04992	0.05196	0.05382	0.05630	0.05929	0.06004	0.06312	0.06503	0.06095	0.06449	0.06572
	0.11774	0.12565	0.12985	0.13280	0.13524	0.13682	0.13752	0.13984	0.13995	0.14079	0.14428	0.14310	0.14392
	-0.23439	-0.24376	-0.25308	-0.26441	-0.27256	-0.28254	-0.29570	-0.29564	-0.31407	-0.32452	-0.31463	-0.32380	-0.33271
	-0.45790	-0.48650	-0.49522	-0.49726	-0.49949	-0.49885	-0.49269	-0.50157	-0.48805	-0.48237	-0.48817	-0.48649	-0.48031
	0.63466	0.64058	0.65444	0.66531	0.67064	0.67167	0.67897	0.67437	0.68529	0.69154	0.70019	0.69225	0.70003
	0.58594	0.59222	0.58714	0.58308	0.58272	0.58581	0.58222	0.59163	0.58234	0.57810	0.56961	0.57869	0.57201
	0.01561	0.01382	0.01299	0.01242	0.01232	0.01304	0.01183	0.01217	0.01163	0.01125	0.01243	0.01165	0.01111
	-0.00667	-0.00404	-0.00343	-0.00325	-0.00330	-0.00372	-0.00327	-0.00344	-0.00326	-0.00315	-0.00409	-0.00331	-0.00317
4S	-0.14686	-0.19484	-0.20783	-0.21808	-0.22740	-0.23612	-0.24401	-0.25346	-0.26201	-0.27018	-0.22896	-0.27797	-0.28519
	-0.00895	-0.01147	-0.01174	-0.01195	-0.01209	-0.01236	-0.01269	-0.01265	-0.01306	-0.01322	-0.01024	-0.01289	-0.01290
	-0.02298	-0.03021	-0.03088	-0.03089	-0.03073	-0.03038	-0.02979	-0.02983	-0.02933	-0.02899	-0.02457	-0.02898	-0.02861
	0.04827	0.06140	0.06315	0.06460	0.06511	0.06599	0.06742	0.06638	0.06931	0.07039	0.05660	0.06909	0.06967
	0.09248	0.12632	0.12757	0.12544	0.12309	0.12001	0.11550	0.11588	0.11072	0.10753	0.08827	0.10654	0.10329
	-0.14391	-0.20261	-0.20740	-0.20734	-0.20439	-0.19948	-0.19642	-0.19204	-0.19223	-0.19091	-0.15341	-0.18751	-0.18659
	-0.30101	-0.36025	-0.35100	-0.33842	-0.32750	-0.31832	-0.30827	-0.30368	-0.29399	-0.28610	-0.23298	-0.28089	-0.27234
	0.69860	0.63445	0.59426	0.58652	0.58293	0.58145	0.57713	0.57734	0.57378	0.57059	0.45551	0.55305	0.55535
	0.40998	0.52586	0.56533	0.56870	0.56740	0.56372	0.56438	0.56115	0.56264	0.56363	0.64751	0.57896	0.57454

TABLE A6.2 (CONTINUED).

	K(2S)	CA(1S)	SC(2D)	TI(3F)	V(4F)	CR(5D)	MN(6S)	FE(5D)	CO(4F)	NI(3F)	CU(2S)	CU(2D)	ZN(1S)
2P	-11.5166	-13.6262	-15.6580	-17.7796	-20.0093	-22.3518	-24.8016	-27.4007	-30.1147	-32.9391	-35.6022	-35.8714	-38.9159
	0.10108	0.09658	0.09484	0.09439	0.09460	0.09918	0.10880	0.10755	0.12165	0.12228	0.10064	0.11347	0.11128
	0.92218	0.91820	0.91930	0.91965	0.91918	0.91817	0.91578	0.91617	0.91373	0.91451	0.92151	0.91752	0.91809
	0.06445	0.07319	0.07261	0.07171	0.07158	0.06797	0.06118	0.06155	0.05016	0.04802	0.06018	0.05273	0.05380
	-0.00184	-0.00147	-0.00143	-0.00105	-0.00079	-0.00043	0.00010	0.00016	0.00047	0.00058	0.00012	0.00040	0.00055
3P	-0.95197	-1.33880	-1.56620	-1.78451	-2.00619	-2.23298	-2.46114	-2.71995	-2.97747	-3.24425	-3.28541	-3.52050	-3.79970
	-0.03119	-0.03183	-0.03222	-0.03278	-0.03344	-0.03565	-0.03973	-0.03975	-0.04565	-0.04630	-0.03783	-0.04318	-0.04260
	-0.30874	-0.33096	-0.34110	-0.34846	-0.35408	-0.35794	-0.35968	-0.36375	-0.36225	-0.36417	-0.36983	-0.36906	-0.37176
	0.27019	0.25841	0.27762	0.28959	0.29825	0.31492	0.33755	0.34472	0.39054	0.40600	0.37596	0.39863	0.39749
	0.83893	0.84895	0.83460	0.82627	0.82027	0.80766	0.78985	0.78443	0.74474	0.73144	0.75940	0.73878	0.74053
3D			-0.34132	-0.43461	-0.49956	-0.55560	-0.62214	-0.62600	-0.64920	-0.67670	-0.45313	-0.70630	-0.74510
			0.39733	0.41599	0.42428	0.43312	0.44479	0.45614	0.46712	0.47550	0.50190	0.47946	0.48398
			0.77686	0.75815	0.75015	0.74225	0.73163	0.72364	0.71495	0.70832	0.69486	0.70542	0.70172