Dependence of Slater—Condon parameters on electron configuration. II. Slater—Condon parameters of elements of the first transition series

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Received 27 July 1977

There are proposed approximative relations for the dependence of values of the Slater—Condon parameters $F^0(4s,4s)$, $F^0(4s,4p)$, $F^0(4s,3d)$, $F^0(4p,3d)$, $F^0(3d,3d)$, $G^1(4s,4p)$, $F^2(3d,3d)$, $F^4(3d,3d)$, $G^2(4s,3d)$, $G^1(4p,3d)$, $F^2(4p,3d)$, and $G^3(4p,3d)$ on electron configuration of atoms (ions) of the first transition series. The proposed functions are useful in LCAO MO SCF methods including the dependence of Hartree—Fock matrix on electron configuration of atoms in molecules.

В работе предложены апроксимативные соотношения для зависимостей величин параметров Слейтера—Кондона $F^0(4s,4s)$, $F^0(4s,4p)$, $F^0(4s,3d)$, $F^0(4p,3d)$, $F^0(3d,3d)$, $G^1(4s,4p)$, $F^2(3d,3d)$, $F^4(3d,3d)$, $G^2(4s,3d)$, $G^1(4p,3d)$, $F^2(4p,3d)$ и $G^3(4p,3d)$ от электронной конфигурации атомов (ионов) первого переходного периода. Предложенные регрессные функции применимые в ЛКАО МО ССП методах с включением зависимости матрицы Хартри—Фока от электронной конфигурации атомов в молекулах.

The semiempirical methods with an explicit inclusion of electron repulsion were up to this time used for calculation of electron structure only for a small number of coordination compounds. At the present state of parametrization they allow a comparison of some physicochemical properties in series of similar molecules. In contrast to IEHT method they give good results for calculations of equilibrium geometries. In spite of a considerable effort expended in this field (see for example review articles [1—3]), the results have not realized expectation, because they are

far from the level of the results of analogical methods applied to organic compounds [4]. A great number of semiempirical methods of this kind mutually differ mainly in using different combinations of some fundamental types of the originally proposed approximations to express different integrals [5].

On the basis of the analysis of atomic spectra [6, 7] it was found that all the monocentric integrals needed for the construction of Hartree—Fock matrix are firmly dependent on the charge and electron configuration of the given atom. The first attempts to regard this fact [8] have shown a considerable improvement of results, mainly for polar systems. Because the bonds in coordination compounds are predominantly strongly polar and a great part of these systems is not electroneutral, the consideration of this fact in parametrization is extraordinarily important.

In the present work there is expressed the dependence of Slater—Condon parameters on electron configuration of atoms and ions of the first transition series.

Method and results

If we wish to calculate values of all monocentric integrals of electron repulsion which arise in the basis of s, p, d atomic orbitals, we need to know values of these integrals of the radial part of atomic orbitals [9]: $F^0(s,s)$, $F^0(s,p)$, $F^0(p,p)$, $F^0(s,d)$, $F^0(p,d)$, $G^1(s,p)$, $F^2(d,d)$, $F^2(p,p)$, $F^4(d,d)$, $G^2(s,d)$, $G^1(p,d)$, $F^2(p,d)$, $G^3(p,d)$, $R^1(s,d,d,d)$, $R^1(s,p,p,d)$, $R^2(s,p,p,d)$. The last three integrals are not the Slater—Condon parameters and we cannot determine them by analysis of atomic spectra, because they do not occur in expressions for energies of atomic terms. From available experimental data there is not possible to determine the Slater—Condon parameters $F^0(4p,p)$ and $F^2(4p,4p)$. The next paper of this series will be devoted to evaluation of parameters $R^1(4s,3d,3d,3d)$, $R^1(4s,4p,4p,3d)$, $R^2(4s,4p,4p,3d)$, $F^0(4p,4p)$, and $F^2(4p,4p)$.

In determination of values of the Slater—Condon parameters F^k and G^k $(k \neq 0)$ *Hinze* and *Jaffé* [10], *Tondello, de Michelis, Oleari,* and *Sipio* [11], and *Anno* and *Teruya* [6] have been engaged. In this work we use the results obtained by *Anno* and *Teruya* [6], because only these are determined systematically with a correct employment of all available spectral data. These values are listed in Tables 6—12 under the symbol Experimental.

The basis for the calculation of values of Slater—Condon parameters of the type F^0 are the energetic balances of reactions of the electron exchange

$$A^{(q+1)+} + A^{(q+1)+} \rightarrow A^{q+} + A^{(q+2)+} \qquad (1)$$

Anno [6, 12] has shown that energetic effect of this electron transmission can be expressed by using the values of the Slater—Condon parameters relevant to the

most negative ion in eqn (*1*). Then the parameters F^0 for atoms and ions with electron configuration $d^\alpha s^\beta p^\gamma$ can be enumerated from the following relations

$$2E^{(q+1)+}(d^\alpha s^{\beta-1} p^\gamma) = E^{q+}(d^\alpha s^\beta p^\gamma) + E^{(q+2)+}(d^\alpha s^{\beta-2} p^\gamma) + \Delta E(s,s) \qquad (2)$$

$$2E^{(q+1)+}(d^\alpha s^\beta p^{\gamma-1}) = E^{q+}(d^\alpha s^\beta p^\gamma) + E^{(q+2)+}(d^\alpha s^\beta p^{\gamma-2}) + \Delta E(p,p) \qquad (3)$$

$$E^{(q+1)+}(d^\alpha s^\beta p^{\gamma-1}) + E^{(q+1)+}(d^\alpha s^{\beta-1} p^\gamma) = E^{q+}(d^\alpha s^\beta p^\gamma) + E^{(q+2)+}(d^\alpha s^{\beta-1} p^{\gamma-1}) + \Delta E(s,p) \qquad (4)$$

$$2E^{(q+1)+}(d^{\alpha-1} s^\beta p^\gamma) = E^{q+}(d^\alpha s^\beta p^\gamma) + E^{(q+2)+}(d^{\alpha-2} s^\beta p^\gamma) + \Delta E(d,d) \qquad (5)$$

$$E^{(q+1)+}(d^\alpha s^{\beta-1} p^\gamma) + E^{(q+1)+}(d^{\alpha-1} s^\beta p^\gamma) = E^{q+}(d^\alpha s^\beta p^\gamma) + E^{(q+2)+}(d^{\alpha-1} s^{\beta-1} p^\gamma + \Delta E(s,d) \qquad (6)$$

$$E^{(q+1)+}(d^\alpha s^\beta p^{\gamma-1}) + E^{(q+1)+}(d^{\alpha-1} s^\beta p^\gamma) = E^{q+}(d^\alpha s^\beta p^\gamma) + E^{(q+2)+}(d^{\alpha-1} s^\beta p^{\gamma-1}) + \Delta E(p,d) \qquad (7)$$

where

$$\Delta E(s,s) = F^0(s,s) \qquad (8)$$

$$\Delta E(p,p) = F^0(p,p) - \frac{2}{25} F^2(p,p) \qquad (9)$$

$$\Delta E(s,p) = F^0(s,p) - \frac{1}{6} G^1(s,p) \qquad (10)$$

$$\Delta E(d,d) = F^0(d,d) - \frac{2}{63} F^2(d,d) - \frac{2}{63} F^4(d,d) \qquad (11)$$

$$\Delta E(s,d) = F^0(s,d) - \frac{1}{10} G^2(s,d) \qquad (12)$$

$$\Delta E(p,d) = F^0(p,d) - \frac{1}{15} G^1(p,d) - \frac{3}{70} G^3(p,d) \qquad (13)$$

We obtain the values ΔE as the difference of average energies of electron configurations on the right and the left side of eqns (*2—7*). We calculate the values F^0 according to eqns (*8—13*) in which we replace F^k and G^k $(k \neq 0)$ by values obtained from approximative expressions according to eqns (*14—16*). Average energies of configurations were enumerated as the weighted mean of energies of individual terms with the weighting factor equal to the multiplicity of the given term. Values of the energies of terms from *Moore*'s spectral tables [13] were used. The obtained values of parameters F^0 are listed in Tables 1—5 under the symbol Experimental.

Table 1. Experimental and calculated values of $F^0(4s,4s)$ [eV]

Z	S	P	D	Experimental	Approximative	Deviation
21	2	0	1	6.1800	5.7272	0.4528
21	2	0	0	6.9831	6.6720	0.3111
22	2	0	2	6.3088	6.2568	0.0520
22	2	0	1	7.9484	8.1725	-0.2241
23	2	0	3	5.6212	6.7326	-1.1114
24	2	0	4	7.4824	7.1547	0.3278
24	2	0	3	6.9740	8.7407	-1.7667
25	2	0	5	7.1132	7.5229	-0.4097
25	2	0	4	10.6826	7.8085	2.8741
26	2	0	6	9.1195	7.8373	1.2822
26	2	0	5	4.8709	6.0654	-1.1945
27	2	0	7	9.4993	8.0979	1.4014
28	2	0	8	7.5045	8.3047	-0.8002
29	2	0	9	8.3186	8.4577	-0.1391

Table 2. Experimental and calculated values of $F^0(4s,4p)$ [eV]

Z	S	P	D	Experimental	Approximative	Deviation
21	1	1	1	5.3397	5.7679	-0.4282
21	1	1	0	6.8433	5.0327	1.8106
22	1	1	2	5.6024	5.9361	-0.3336
22	1	1	1	7.7550	7.2743	0.4807
22	1	1	0	6.9889	8.6126	-1.6237
23	1	1	3	5.1129	6.1012	-0.9883
23	1	1	2	7.9204	8.4226	-0.5022
24	1	1	4	6.2328	6.2634	-0.0306
25	1	1	5	6.3896	6.4225	-0.0328
25	1	1	4	10.9592	7.4393	3.5199
26	1	1	6	7.3148	6.5787	0.7362
26	1	1	5	3.2460	5.3077	-2.0617
27	1	1	7	8.1508	6.7318	1.4190
28	1	1	8	5.8453	6.8819	-1.0366
29	1	1	9	7.2337	7.0290	0.2047

Table 3. Experimental and calculated values of $F^0(4s,3d)$ [eV]

Z	S	P	D	Experimental	Approximative	Deviation
21	1	0	2	7.2014	6.8226	0.3788
21	1	1	1	8.0473	8.5723	-0.5250
21	2	0	1	7.6126	8.5723	-0.9597
21	1	0	1	8.8609	8.9526	-0.0917
22	1	0	3	7.4075	6.5746	0.8330
22	1	1	2	8.2600	7.8613	0.3987

Table 3 (Continued)

Z	S	P	D	Experimental	Approximative	Deviation
22	2	0	2	7.9600	7.8613	0.0987
22	1	0	2	9.9556	9.7909	0.1647
22	1	1	1	11.0665	9.8338	1.2327
22	1	0	1	10.0525	10.6689	-0.6163
23	1	0	4	6.5738	7.0628	-0.4890
23	1	1	3	8.5437	8.1125	0.4312
23	1	0	3	11.1158	10.6159	0.5001
24	1	0	5	8.3758	7.9486	0.4273
24	1	1	4	10.0181	8.9871	1.0311
24	1	0	4	9.5173	11.0886	-1.5713
25	1	0	6	8.5111	8.8929	-0.3818
25	1	1	5	8.7515	10.1461	-1.3946
25	2	0	5	7.9815	10.1461	-2.1646
25	1	0	5	12.3127	10.8704	1.4423
26	1	1	6	11.0971	11.2509	-0.1539
26	1	0	7	8.5575	9.5572	-0.9996
26	2	0	6	11.5655	11.2509	0.3146
26	1	0	6	9.1784	9.6223	-0.4440
27	1	1	7	13.2015	11.9626	1.2388
27	1	0	8	10.4773	9.6024	0.8749
27	2	0	7	12.9971	11.9626	1.0345
28	1	0	9	8.9500	8.6898	0.2602
29	1	0	10	6.1932	6.4806	-0.2873
29	1	1	9	10.3495	10.8514	-0.5018
29	2	0	9	10.7708	10.8514	-0.0806

Table 4. Experimental and calculated values of $F^0(4p,3d)$ [eV]

Z	S	P	D	Experimental	Approximative	Deviation
21	1	1	1	6.4936	7.2289	-0.7354
21	0	1	2	6.0789	5.6066	0.4723
21	0	1	1	7.7183	7.6716	0.0466
22	0	1	3	6.2383	5.6072	0.6311
22	1	1	2	6.7915	6.9682	-0.1767
22	0	1	2	8.6755	8.7064	-0.0309
22	1	1	1	9.9658	8.9757	0.9902
22	0	1	1	9.0160	8.5111	-0.4951
23	0	1	4	5.3765	5.9198	-0.5434
23	1	1	3	7.1225	7.0859	0.0366
23	0	1	3	9.7112	9.3330	0.3782
24	0	1	5	6.7753	6.4450	0.3303
24	0	1	4	8.0363	9.4521	-1.4158
25	0	1	6	7.1283	7.0832	0.0451
25	1	1	5	10.5515	8.9642	1.5873
25	0	1	5	6.1997	8.0583	-1.8586
26	1	1	6	9.5608	8.7141	0.8467

Table 4 (Continued)

Z	S	P	D	Experimental	Approximative	Deviation
26	0	1	7	7.0211	7.7349	-0.7138
26	0	1	6	7.2042	7.7696	-0.5655
27	0	1	8	9.0666	8.3006	0.7660
27	1	1	7	11.2869	9.3502	1.9367
28	0	1	9	6.9778	8.6808	-1.7029
29	0	1	10	9.9863	8.7760	1.2103
29	1	1	9	9.1259	10.1654	-1.0395

Table 5. Experimental and calculated values of $F^0(3d,3d)$ [eV]

Z	S	P	D	Experimental	Approximative	Deviation
21	1	0	2	11.4972	11.6104	-0.1132
21	0	0	3	8.5941	8.1992	0.3949
21	0	1	2	11.4998	11.2407	0.2591
21	0	0	2	13.1765	13.5472	-0.3707
22	1	0	3	11.8764	11.5835	0.2928
22	0	0	4	9.4317	8.7279	0.7038
22	0	1	3	11.9958	11.2138	0.7820
22	1	1	2	12.8083	14.6250	-1.8168
22	0	0	3	14.4253	13.5203	0.9050
22	1	0	2	16.0585	16.9315	-0.8730
22	0	1	2	15.8511	16.5618	-0.7107
22	0	0	2	16.1863	18.8682	-2.6820
23	0	0	5	9.2002	9.5922	-0.3920
23	1	0	4	11.0697	11.8922	-0.8225
23	0	1	4	11.2984	11.5226	-0.2242
23	0	0	4	15.6077	13.8290	1.7787
23	1	0	3	18.0096	16.6846	1.3250
23	0	1	3	17.8198	16.3150	1.5049
24	0	0	6	9.4752	10.7920	-1.3169
24	1	0	5	13.6595	12.5366	1.1230
24	0	1	5	13.5326	12.1669	1.3657
24	0	0	5	14.7789	14.4733	0.3056
24	1	0	4	16.6278	16.7734	-0.1456
24	0	1	4	16.3102	16.4037	-0.0935
25	1	0	6	12.7520	13.5165	-0.7645
25	0	0	7	10.9734	12.3275	-1.3542
25	0	1	6	13.1410	13.1468	-0.0058
25	0	0	6	16.5399	15.4533	1.0866
25	1	0	5	20.3098	17.1978	3.1120
26	0	0	8	11.6171	14.1986	-2.5815
26	1	0	7	14.3117	14.8320	-0.5203
26	0	1	7	14.7360	14.4624	0.2737
26	0	0	7	14.9026	16.7688	-1.8662

Table 5 (Continued)

Z	S	P	D	Experimental	Approximative	Deviation
26	0	1	6	13.3202	17.5881	-4.2678
27	0	0	9	13.4171	16.4054	-2.9883
27	1	0	8	17.1618	16.4832	0.6786
27	0	1	8	17.5036	16.1135	1.3900
28	0	0	10	25.5080	18.9477	6.5603
28	1	0	9	16.9944	18.4699	-1.4755
28	0	1	9	15.9700	18.1003	-2.1303

Table 6. Experimental and calculated values of $G^1(4s,4p)$ [eV]

Z	S	P	D	Experimental	Approximative	Deviation
21	1	1	1	1.5001	1.4674	0.0327
21	1	1	0	3.0622	3.0622	0.0000
22	1	1	2	1.6241	1.6854	-0.0613
22	1	1	1	2.9631	2.9631	0.0000
23	1	1	3	1.8721	1.8059	0.0662
23	1	1	2	3.1118	3.1118	0.0000
24	1	1	4	1.7853	1.8971	-0.1118
25	1	1	5	2.3432	2.0908	0.2524
25	1	1	4	3.4714	3.4714	0.0000
26	1	1	6	3.0208	3.3681	-0.3473
26	1	1	5	3.4466	3.4466	0.0000
27	1	1	7	2.8143	2.5522	0.2621
27	1	1	6	1.7605	1.7605	0.0000
28	1	1	8	2.4052	2.5081	-0.1029
29	1	1	9	2.5663	2.5497	0.0166
29	1	1	8	3.9301	3.9301	0.0000

Table 7. Experimental and calculated values of $F^2(3d,3d)$ [eV]

Z	S	P	D	Experimental	Approximative	Deviation
21	0	0	3	3.2730	3.2025	0.0705
21	1	0	2	3.6573	3.6026	0.0547
21	0	1	2	4.1408	3.9748	0.1660
21	0	0	2	4.4756	4.6128	-0.1372
22	0	0	4	3.6821	3.6480	0.0341
22	1	0	3	4.5996	4.6718	-0.0723
22	0	1	3	4.8971	5.1166	-0.2195
22	2	0	2	5.5666	5.6608	-0.0942

Table 7 (Continued)

Z	S	P	D	Experimental	Approximative	Deviation
22	1	1	2	5.6038	5.8950	-0.2912
22	0	0	3	5.2070	5.1973	0.0097
22	1	0	2	6.4344	6.1560	0.2784
22	0	1	2	6.2113	6.2483	-0.0370
22	0	0	2	6.6700	6.6512	0.0188
23	0	0	5	3.5211	3.5211	0.0000
23	1	0	4	5.2938	5.4281	-0.1342
23	0	1	4	5.8021	5.6017	0.2004
23	2	0	3	6.2980	6.4038	-0.1058
23	1	1	3	6.9427	6.7911	0.1513
23	0	0	4	5.4178	5.6205	-0.2027
23	1	0	3	7.0047	6.6367	0.3680
23	0	1	3	6.8807	6.8823	-0.0016
23	1	1	2	8.3189	8.1794	0.1395
23	0	0	3	6.8807	6.8696	0.0111
23	1	0	2	8.3189	8.3469	-0.0281
23	0	1	2	8.3189	8.2400	0.0788
23	0	0	2	8.4429	8.5495	-0.1067
24	0	0	6	4.9343	4.9343	0.0000
24	1	0	5	6.2113	6.1917	0.0196
24	0	1	5	6.2980	6.4855	0.1875
24	2	0	4	7.8726	7.5669	0.3057
24	1	1	4	7.8354	7.7459	0.0895
24	0	0	5	6.5088	6.3409	0.1679
24	1	0	4	7.5006	7.6423	-0.1417
24	0	1	4	7.5998	7.6794	-0.0796
24	2	0	3	8.2941	8.3919	-0.0978
24	0	0	4	7.7486	7.7177	0.0309
24	1	0	3	8.2569	8.5078	-0.2509
24	0	1	3	8.8272	8.6168	0.2103
24	0	0	3	8.4800	8.6237	-0.1437
24	1	0	2	10.3273	10.2921	0.0352
24	0	1	2	9.9926	10.0487	-0.0561
25	0	0	7	5.0087	5.0087	0.0000
25	1	0	6	7.8974	7.6140	0.2834
25	0	1	6	7.7362	7.6802	0.0560
25	2	0	5	8.1825	8.1627	0.0198
25	1	1	5	8.3437	8.5064	-0.1627
25	0	0	6	7.0791	7.4184	-0.3393
25	1	0	5	8.2693	8.3238	-0.0595
25	0	1	5	8.6412	8.5256	0.1156
25	2	0	4	9.5958	9.6585	-0.0627
25	1	1	4	9.5958	9.7454	-0.1495
25	0	0	5	8.5668	8.4849	0.0819
25	1	0	4	9.5958	9.7458	-0.1500
25	0	1	4	9.5958	9.6907	-0.0949
25	0	0	4	10.9472	10.7361	0.2111
25	1	0	3	10.1537	9.8331	0.3206
25	0	1	3	10.6125	10.7530	-0.1405

Table 7 (Continued)

Z	S	P	D	Experimental	Approximative	Deviation
26	0	0	8	6.1864	6.1864	0.0000
26	1	0	7	7.5626	7.5839	-0.0213
26	0	1	7	7.7362	7.7951	-0.0590
26	2	0	6	8.6412	8.8898	-0.2485
26	1	1	6	8.9388	9.0321	-0.0933
26	0	0	7	7.6122	7.5318	0.0804
26	1	0	6	8.8148	8.7882	0.0265
26	0	1	6	8.9140	8.7886	0.1254
26	2	0	5	9.7322	9.7330	-0.0008
26	1	1	5	10.3397	10.0108	0.3289
26	0	0	6	8.8768	8.6867	0.1900
26	1	0	5	9.8189	9.9881	-0.1692
26	0	1	5	10.0298	10.1240	-0.0942
26	0	0	5	10.1785	10.2433	-0.0647
26	0	1	4	11.5919	11.5577	0.0341
27	1	0	8	7.9965	8.0090	-0.0125
27	0	1	8	8.0461	8.0176	0.0285
27	2	0	7	9.1991	9.1019	0.0972
27	1	1	7	9.5958	9.3974	0.1985
27	0	0	8	8.1701	8.1859	-0.0158
27	1	0	7	8.7156	9.1793	-0.4637
27	0	1	7	9.2859	9.3328	-0.0469
27	2	0	6	10.9224	10.7838	0.1386
27	1	1	6	10.9224	10.8684	0.0540
27	0	0	7	9.4719	9.2567	0.2152
27	1	0	6	10.7612	10.8118	-0.0506
27	0	1	6	10.6125	10.7544	-0.1420
28	2	0	8	9.8934	9.7714	0.1220
28	1	1	8	9.6206	9.8543	-0.2336
28	1	0	8	10.2157	10.0666	0.1491
28	0	1	8	10.1413	10.0075	0.1338
28	0	0	8	10.1909	10.3618	-0.1709
28	1	0	8	11.0836	10.9911	0.0925
28	0	1	8	10.9844	11.0768	-0.0924
29	2	0	8	11.5051	11.5490	-0.0439
29	1	1	8	11.5051	11.5360	-0.0309
29	1	0	8	11.8770	11.9045	-0.0275
29	0	1	8	11.8522	11.7496	0.1026

Table 8. Experimental and calculated values of $F^4(3d,3d)$ [eV]

Z	S	P	D	Experimental	Approximative	Deviation
21	0	0	3	1.2398	1.2371	0.0026
21	1	0	2	1.8101	2.1720	-0.3619
21	0	1	2	2.1324	2.0764	0.0560

Table 8 (Continued)

Z	S	P	D	Experimental	Approximative	Deviation
21	0	0	2	2.8143	2.5877	0.2266
22	0	0	4	1.8845	1.6353	0.2492
22	1	0	3	2.9501	2.9385	0.0122
22	0	1	3	3.0994	3.0167	0.0828
22	2	0	2	3.6821	3.6041	0.0780
22	1	1	2	3.4218	3.6191	-0.1973
22	0	0	3	2.9383	3.1908	-0.2526
22	1	0	2	4.4756	3.9331	0.5425
22	0	1	2	3.9921	3.9745	0.0175
22	0	0	2	4.1160	4.2621	-0.1460
23	0	0	5	1.6613	2.2327	-0.5713
23	1	0	4	3.2482	3.2212	0.0270
23	0	1	4	3.4466	3.3705	0.0761
23	2	0	3	4.3888	4.1942	0.1946
23	1	1	3	4.2524	4.3240	-0.0716
23	0	0	4	3.3598	3.3824	-0.0226
23	1	0	3	4.5252	4.3283	0.1969
23	0	1	3	4.2772	4.4846	-0.2074
23	1	1	2	5.2318	5.1566	0.0752
23	0	0	3	4.2772	4.4625	-0.1853
23	1	0	2	5.2318	5.2743	-0.0424
23	0	1	2	5.2318	5.3938	-0.1620
23	0	0	2	5.3806	5.4851	-0.1045
24	0	0	6	3.0498	3.0308	0.0190
24	1	0	5	3.9797	3.7214	0.2582
24	0	1	5	4.1532	3.8546	0.2986
24	2	0	4	4.5624	4.5137	0.0486
24	1	1	4	4.6987	4.6829	0.0159
24	0	0	5	3.9673	3.8363	0.1310
24	1	0	4	4.5624	4.5555	0.0059
24	0	1	4	4.8599	4.7520	0.1079
24	2	0	3	4.9715	5.4615	-0.4900
24	0	0	4	4.8847	4.5992	0.2855
24	1	0	3	5.1946	5.4771	-0.2825
24	0	1	3	5.8517	5.6797	0.1720
24	0	0	3	5.4054	5.4928	-0.0874
24	1	0	2	6.5832	6.5982	-0.0150
24	0	1	2	7.0295	6.7640	0.2655
25	0	0	7	4.1780	3.7214	0.4566
25	1	0	6	4.2028	4.3931	-0.1902
25	0	1	6	4.1780	4.4387	-0.2606
25	2	0	5	4.6987	5.0070	-0.3083
25	1	1	5	5.2070	5.1553	0.0517
25	0	0	6	4.4136	4.4789	-0.0653
25	1	0	5	4.9591	5.0342	-0.0751
25	0	1	5	4.8971	5.2089	-0.3118
25	2	0	4	6.0377	5.8140	0.2246
25	1	1	4	6.0377	6.0247	0.0130
25	0	0	5	5.0707	5.0613	0.0093

Table 8 (Continued)

Z	S	P	D	Experimental	Approximative	Deviation
25	1	0	4	6.0377	5.7691	0.2686
25	0	1	4	6.0377	6.0061	0.0316
25	0	0	4	5.8145	5.7241	0.0905
25	1	0	3	6.9427	6.7946	0.1482
25	0	1	3	6.9179	7.0386	-0.1207
26	0	0	8	4.1036	4.1724	-0.0688
26	1	0	7	4.7607	5.0351	-0.2744
26	0	1	7	4.6987	4.9371	-0.2384
26	2	0	6	5.7773	5.5894	0.1879
26	1	1	6	5.7030	5.6724	0.0306
26	0	0	7	5.2566	5.0817	0.1749
26	1	0	6	5.5294	5.6494	-0.1200
26	0	1	6	5.9013	5.7588	0.1426
26	2	0	5	5.9633	6.3217	-0.3584
26	1	1	5	6.5832	6.5338	0.0494
26	0	0	6	5.7773	5.7093	0.0680
26	1	0	5	6.6080	6.3230	0.2850
26	0	1	5	6.6080	6.5615	0.0465
26	0	0	5	6.1369	6.3243	-0.1874
26	0	1	4	7.3766	7.5673	-0.1907
27	1	0	8	5.9633	5.6713	0.2921
27	0	1	8	5.2318	5.3893	-0.1574
27	2	0	7	6.2609	6.1335	0.1273
27	1	1	7	6.2609	6.1223	0.1386
27	0	0	8	5.4798	5.6410	-0.1612
27	1	0	7	5.6658	6.2472	-0.5815
27	0	1	7	6.5708	6.2624	0.3084
27	2	0	6	7.0295	6.8320	0.1975
27	1	1	6	7.0295	7.0282	0.0013
27	0	0	7	6.3972	6.3610	0.0362
27	1	0	6	7.0295	6.9591	0.0704
27	0	1	6	7.1659	7.1817	-0.0158
28	2	0	8	6.6080	6.7426	-0.1347
28	1	1	8	6.5832	6.6238	-0.0406
28	1	0	8	7.2279	6.9036	0.3243
28	0	1	8	7.0667	6.8112	0.2554
28	0	0	8	6.7940	7.0645	-0.2705
28	1	0	7	7.6494	7.5247	0.1247
28	0	1	7	7.5006	7.7295	-0.2288
29	2	0	8	7.4138	7.5537	-0.1398
29	1	1	8	7.6618	7.7280	-0.0662
29	1	0	8	8.1949	8.0609	0.1340
29	0	1	8	8.2941	8.2616	0.0325

Table 9. Experimental and calculated values of $G^2(4s,3d)$ [eV]

Z	S	P	D	Experimental	Approximative	Deviation
21	1	0	2	0.7277	0.6728	0.0550
21	1	1	1	0.8282	0.8228	0.0054
21	1	0	1	0.7550	0.9271	-0.1721
22	1	0	3	0.7687	0.7517	0.0170
22	1	1	2	0.3124	0.4298	-0.1173
22	1	0	2	0.9422	0.9901	-0.0479
22	1	1	1	1.3390	1.2915	0.0475
22	1	0	1	1.0625	0.9427	0.1198
23	1	0	4	0.7736	0.7876	-0.0140
23	1	1	3	1.0300	1.1178	-0.0875
23	1	0	3	0.9844	0.9408	0.0436
23	1	1	2	1.0079	0.8647	0.1432
23	1	0	2	1.0873	1.0666	0.0207
23	1	0	1	1.1332	1.1097	0.0235
24	1	0	5	0.6472	0.6227	0.0244
24	1	1	4	0.9831	0.8513	0.1318
24	1	0	4	0.8182	0.9276	-0.1094
24	1	0	3	1.0501	1.0104	0.0397
24	1	0	2	1.2286	1.1859	-0.0528
25	1	0	6	0.7575	0.7766	-0.0191
25	1	1	5	0.8121	0.9604	-0.1483
25	1	0	5	0.9769	0.8781	0.0988
25	1	1	4	1.2770	1.2397	0.0372
25	1	0	4	1.1071	1.1467	-0.0396
25	1	0	3	1.2286	1.2444	-0.0158
26	1	0	7	0.8232	0.8169	0.0063
26	1	1	6	1.3885	1.1967	0.1918
26	1	0	6	0.9683	1.1154	-0.1472
26	1	1	5	1.1369	1.1923	-0.0555
26	1	0	5	1.1084	1.0354	0.0730
27	1	0	8	0.7860	0.7860	0.0000
27	1	1	7	0.3806	0.4561	-0.0755
27	1	0	7	0.9707	0.9141	0.0566
27	1	1	6	1.1641	1.1990	-0.0349
27	1	0	6	1.1530	1.1377	0.0153
28	1	0	9	0.8306	0.8309	-0.0003
28	1	1	8	1.2125	1.1665	0.0460
28	1	0	8	0.9447	0.9880	-0.0433
28	1	0	7	1.2113	1.2017	0.0095
29	1	1	9	0.5529	0.5554	-0.0025
29	1	0	9	1.1208	1.1181	-0.0027
29	1	1	8	1.0538	1.0791	-0.0253

Table 10. Experimental and calculated values of $G^1(4p,3d)$ [eV]

Z	S	P	D	Experimental	Approximative	Deviation
21	0	1	2	0.6496	0.6483	0.0013
21	1	1	1	0.7005	0.7054	-0.0049
21	0	1	1	0.7067	0.7024	0.0043
22	0	1	3	0.4922	0.4964	-0.0042
22	1	1	2	0.9075	0.9237	-0.0162
22	0	1	2	0.6348	0.6215	0.0132
22	1	1	1	0.7426	0.6990	0.0436
22	0	1	1	0.8096	0.8504	-0.0408
23	0	1	4	0.4674	0.4674	0.0000
23	1	1	3	0.6422	0.6472	-0.0050
23	0	1	3	0.6050	0.5702	0.0349
23	1	1	2	0.6199	0.6698	-0.0499
23	0	1	2	0.8133	0.7788	0.0345
23	0	1	1	0.9422	0.9422	0.0000
24	0	1	5	0.6112	0.5906	0.0206
24	1	1	4	0.6918	0.6637	0.0281
24	0	1	4	0.5802	0.6906	-0.1104
24	0	1	3	0.7897	0.7554	0.0343
24	0	1	2	0.9174	0.9174	0.0000
25	0	1	6	0.1537	0.1947	-0.0410
25	1	1	5	0.6323	0.5382	0.0941
25	0	1	5	0.5963	0.5787	0.0176
25	1	1	4	0.8840	0.9106	-0.0266
25	0	1	4	0.7972	0.8077	-0.0105
25	0	1	3	0.9311	0.9311	0.0000
26	0	1	7	0.3037	0.2670	0.0367
26	1	1	6	0.2913	0.3891	-0.0977
26	0	1	6	0.5021	0.4847	0.0175
26	1	1	5	0.7662	0.8043	-0.0381
26	0	1	5	0.7501	0.6947	0.0544
26	0	1	4	0.8964	0.8964	0.0000
27	0	1	8	0.3930	0.4092	-0.0162
27	1	1	7	0.3546	0.3534	0.0012
27	0	1	7	0.5430	0.5166	0.0265
27	1	1	6	0.7277	0.6200	0.1077
27	0	1	6	0.4786	0.5846	-0.1061
28	0	1	9	0.3732	0.3702	0.0000
28	1	1	8	0.3818	0.4246	-0.0428
28	0	1	8	0.5653	0.5245	0.0408
28	0	1	7	0.7277	0.7322	-0.0045
29	1	1	9	0.6968	0.6533	0.0435
29	0	1	9	0.6149	0.6590	-0.0717
29	1	1	8	0.6484	0.6849	-0.0365
29	0	1	8	0.7488	0.7110	0.0378

Table 11. Experimental and calculated values of $F^2(4p,3d)$ [eV]

Z	S	P	D	Experimental	Approximative	Deviation
21	0	1	2	0.8368	0.8041	0.0327
21	1	1	1	1.3637	1.3551	0.0087
21	0	1	1	1.0501	1.0304	0.0197
22	0	1	3	0.6980	0.7804	-0.0824
22	1	1	2	1.6985	1.6365	0.0619
22	0	1	2	1.2646	1.3384	-0.0738
22	1	1	1	1.7109	1.7046	0.0062
22	0	1	1	1.9216	1.9911	-0.0695
23	0	1	4	0.9447	0.7379	0.2068
23	1	1	3	1.3885	1.5265	-0.1379
23	0	1	3	1.4257	1.4411	-0.0154
23	1	1	2	2.0704	2.1413	-0.0709
23	0	1	2	2.4052	2.1984	0.2068
23	0	1	1	2.5291	2.4841	0.0451
24	0	1	5	0.2752	0.5386	-0.3634
24	1	1	4	1.4133	1.2987	0.1146
24	0	1	4	1.5869	1.4345	0.1524
24	0	1	3	2.1944	2.2640	-0.0696
24	0	1	2	2.5663	2.6940	-0.1277
25	0	1	6	0.9931	0.6332	0.3599
25	1	1	5	0.9683	1.1336	-0.1654
25	0	1	5	1.4629	1.3993	0.0636
25	1	1	4	2.3184	2.1300	0.1884
25	0	1	4	2.0952	2.2434	-0.1481
25	0	1	3	3.0126	2.8925	0.1201
26	0	1	7	0.6224	0.7749	-0.1525
26	1	1	6	1.2770	1.2034	0.0734
26	0	1	6	1.2770	1.4871	-0.2101
26	1	1	5	2.1572	2.1650	-0.0078
26	0	1	5	2.1076	2.2867	-0.1791
26	0	1	4	3.1242	3.1617	-0.0375
27	0	1	8	0.7798	0.7914	-0.0116
27	1	1	7	1.5001	1.3500	0.1501
27	0	1	7	1.5745	1.5973	-0.0228
27	1	1	6	2.2192	2.3933	-0.1741
27	0	1	6	2.9135	2.4562	0.4573
28	0	1	9	0.7501	0.7298	0.0202
28	1	1	8	1.0625	1.1707	-0.1082
28	0	1	8	1.5745	1.4634	0.1111
28	0	1	7	2.2936	2.4843	-0.1907
29	1	1	9	1.3266	1.3240	0.0025
29	0	1	9	1.9340	1.9587	-0.0247
29	1	1	8	2.2936	2.2353	0.0582
29	0	1	8	2.2812	2.2881	-0.0069

Table 12. Experimental and calculated values of $G^3(4p,3d)$ [eV]

Z	S	P	D	Experimental	Approximative	Deviation
21	0	1	2	0.0811	0.1636	-0.0825
21	1	1	1	0.2740	0.3623	-0.0883
21	0	1	1	0.0807	0.0610	0.0197
22	1	1	2	1.2770	1.0210	0.2560
22	0	1	2	0.2095	0.1937	0.0158
22	1	1	1	0.1163	0.0271	0.0892
22	0	1	1	0.4600	0.4737	-0.0137
23	0	1	4	-0.2318	-0.2019	-0.0300
23	1	1	3	0.2120	0.1616	0.0504
23	0	1	3	0.3025	0.2555	0.0470
23	1	1	2	0.4513	0.7182	-0.2669
23	0	1	2	0.4500	0.4910	-0.0409
23	0	1	1	0.7154	0.7439	-0.0285
24	0	1	5	0.1438	0.1809	-0.0371
24	1	1	4	0.0368	0.2119	-0.1751
24	0	1	4	0.5430	0.2482	0.2948
24	0	1	3	0.6112	0.6356	-0.0244
24	0	1	2	0.7339	0.6119	0.1220
25	0	1	6	0.6162	0.6205	-0.0043
25	1	1	5	0.3037	0.2007	0.1030
25	0	1	5	0.4414	0.4275	0.0138
25	1	1	4	0.4352	0.3850	0.0501
25	0	1	4	0.4922	0.7257	-0.2335
25	0	1	3	0.6782	0.7162	-0.0380
26	0	1	7	0.4364	0.4293	0.0071
26	1	1	6	0.0109	0.1872	-0.1763
26	0	1	6	0.5653	0.3903	0.1750
26	1	1	5	0.7017	0.6183	0.0834
26	0	1	5	0.8083	1.0017	-0.1933
26	0	1	4	0.9050	0.7872	0.1179
27	0	1	8	0.2802	0.2802	0.0000
27	1	1	7	0.8864	0.7877	0.0987
27	0	1	7	0.3806	0.5007	-0.1201
27	1	1	6	0.6137	0.6107	0.0030
27	0	1	6	0.8492	0.8225	0.0267
28	0	1	9	0.4029	0.4036	-0.0007
28	1	1	8	-0.0622	0.0106	-0.0728
28	0	1	8	0.5195	0.4412	0.0783
28	0	1	7	0.6670	0.6648	0.0022
29	1	1	9	0.8592	0.8548	0.0044
29	0	1	9	0.9112	0.9154	-0.0041
29	1	1	8	0.7773	0.7362	0.0411
29	0	1	8	0.8369	0.8800	-0.0431

In the framework of LCAO MO approximation electron configuration of atoms in molecules acquires as a rule noninteger values $d^v s^x p^y$, where v, x, y are nonnegative real numbers obtained by population analysis. Thus, if we want to use the configurationally dependent values of monocentric integrals, obtained by the analysis of atomic spectra in MO calculation of electron structure of molecules, we must approximate the discrete functions with the continuous ones. Then we consider individual monocentric integrals to be functions of continuous arguments which are represented by populations of the individual levels of the valence sphere of an atom, or functions of atomic charge and its atomic number. The dependence on the atomic number is included to render the maximum possible number of known experimental data in the regression.

The most suitable polynomial functions are of the following types

$$F(Z,Q)=\sum_{i=0}^{N_Z}\sum_{j=0}^{N_Q}B_{ij}Z^iQ^j \tag{14}$$

$$F(Z,Q)=\sum_{i=0}^{N_Z}\sum_{j=0}^{N_Q}B_{ij}Z^i(Q+1)^j \tag{15}$$

$$F(Z,v,Q)=\sum_{i=0}^{N_Z}\sum_{j=0}^{N_d}B_{ijo}Z^iv^j+$$
$$+\sum_{i=0}^{N_Z}\sum_{k=1}^{N_Q}B_{iok}Z^iQ^k+\sum_{j=1}^{N_d}\sum_{k=1}^{N_Q}B_{ojk}v^jQ^k \tag{16}$$

$$F(Z,v,x,y)=\sum_{i=0}^{N_Z}\sum_{j=0}^{N_d}B_{ijoo}Z^iv^j+\sum_{i=0}^{N_Z}\sum_{k=1}^{N_s}B_{iok o}Z^ix^k+$$
$$+\sum_{i=0}^{N_Z}\sum_{l=1}^{N_p}B_{iool}Z^iy^l+\sum_{j=1}^{N_d}\sum_{k=1}^{N_s}B_{ojko}v^jx^k+$$
$$+\sum_{k=1}^{N_d}\sum_{l=1}^{N_p}B_{ookl}x^ky^l \tag{17}$$

$$F(Z,v,x,y)=\sum_{i=0}^{N_Z}\sum_{j=0}^{N_d}B_{ijoo}Z^iv^j+\sum_{i=0}^{N_Z}\sum_{k=1}^{N_s}B_{iok o}Z^ix^k+$$
$$+\sum_{i=0}^{N_Z}\sum_{l=1}^{N_p}B_{iool}Z^i(y+1)^l+\sum_{j=1}^{N_d}\sum_{k=1}^{N_s}B_{ojko}v^jx^k+$$
$$+\sum_{j=1}^{N_d}\sum_{l=1}^{N_p}B_{ookl}x^k(y+1)^l \tag{18}$$

Z is the atomic number, Q is the atomic charge, x, y, v are the populations of s, p, d valence orbitals, respectively. The constants B were determined by the least-squares method and the optimum degrees of polynomials N_Z, N_Q, N_s, N_p, N_d were determined by the maximization of the correlation coefficient.

Table 13. Numerical values of B_{ij}'s for function $F^0(4s,4s)$ [eV]

i	j	B_{ij}
0	0	-0.17824361×10^2
1	0	0.16864641×10^1
2	0	$-0.26902984 \times 10^{-1}$
0	1	-0.19432986×10^3
1	1	0.17248220×10^2
2	1	-0.37854408
Correlation coefficient		0.6164
Standard deviation		1.4928

Table 14. Numerical values of B_{ij}'s for function $F^0(4s,4p)$ [eV]

i	j	B_{ij}
0	0	0.15419761×10^1
1	0	0.23280751
2	0	$-0.15034334 \times 10^{-2}$
0	1	-0.29613501×10^3
1	1	0.25514732×10^2
2	1	-0.54514638
Correlation coefficient		0.5746
Standard deviation		1.7108

Table 15. Numerical values of B_{ijk}'s for function $F^0(4s,3d)$ [eV]

i	j	k	B_{ijk}
0	0	0	0.16556008×10^2
1	0	0	-0.29858570
0	1	0	-0.18108587×10^2
0	2	0	0.11677389×10^1
0	0	1	-0.11239755×10^2
1	1	0	0.78158675
1	2	0	$-0.56470560 \times 10^{-1}$
1	0	1	0.45475789
0	1	1	0.25578768×10^1
0	2	1	-0.48777289
Correlation coefficient			0.8750
Standard deviation			1.0347

Table 16. Numerical values of B_{ijk}'s for function $F^0(4p,3d)$ [eV]

i	j	k	B_{ijk}
0	0	0	-0.12591724×10^2
1	0	0	0.10279628×10^1
0	1	0	-0.60386716×10^1
0	2	0	0.42039315
0	0	1	-0.34923361×10^1
1	1	0	0.20000012
1	2	0	$-0.16584784 \times 10^{-1}$
1	0	1	$0.92659630 \times 10^{-1}$
0	1	1	0.23824099×10
0	2	1	-0.39321501
Correlation coefficient			0.7958
Standard deviation			1.2620

Table 17. Numerical values of B_{ijkl}'s for function $F^0(3d,3d)$ [eV]

i	j	k	l	B_{ijkl}
0	0	0	0	-0.13664214×10^3
1	0	0	0	0.10050080×10^2
2	0	0	0	-0.10997682
0	1	0	0	-0.67368617×10^1
0	2	0	0	0.27778017
0	0	1	0	-0.19367667×10^1
0	0	0	1	-0.23064341×10^1
Correlation coefficient				0.8293
Standard deviation				2.0562

Table 18. Numerical values of B_{ij}'s for function $G^1(4s,4p)$ [eV]

i	j	B_{ij}
0	0	-0.52582741×10^6
1	0	0.13131437×10^6
2	0	-0.13639073×10^5
3	0	0.75412728×10^3
4	0	-0.23409239×10^2
5	0	0.38677523
6	0	$-0.26571468 \times 10^{-2}$
0	1	0.58540942×10^6
1	1	-0.14613573×10^6

Table 18 (Continued)

i	j	B_{ij}
2	1	0.15170134 x 10^5
3	1	- 0.83819350 x 10^3
4	1	0.25996794 x 10^2
5	1	- 0.42910668
6	1	0.29447050 x 10^{-2}
Correlation coefficient		0.9844
Standard deviation		0.3090

Table 19. Numerical values of B_{ijkl}'s for function $F^2(3d,3d)$ [eV]

i	j	k	l	B_{ijkl}
0	0	0	0	- 0.32054076 x 10^6
1	0	0	0	0.37486733 x 10^5
2	0	0	0	- 0.14530535 x 10^4
3	0	0	0	0.18667090 x 10^2
0	1	0	0	0.51733593 x 10^6
0	2	0	0	- 0.33069577 x 10^6
0	3	0	0	0.10707995 x 10^6
0	4	0	0	- 0.18535566 x 10^5
0	5	0	0	0.16287400 x 10^4
0	6	0	0	- 0.56937537 x 10^2
0	0	1	0	- 0.95921571 x 10^2
0	0	0	1	- 0.10955426 x 10^3
1	1	0	0	- 0.60760009 x 10^5
1	2	0	0	0.38994653 x 10^5
1	3	0	0	- 0.12670171 x 10^5
1	4	0	0	0.21996269 x 10^4
1	5	0	0	- 0.19377143 x 10^3
1	6	0	0	0.67890749 x 10^1
1	0	1	0	0.16590080 x 10^2
1	0	0	1	0.10185466 x 10^2
2	1	0	0	0.23666407 x 10^4
2	2	0	0	- 0.15257084 x 10^4
2	3	0	0	0.49763330 x 10^3
2	4	0	0	- 0.86667455 x 10^2
2	5	0	0	0.76552729 x 10^1
2	6	0	0	- 0.26883875
2	0	1	0	- 0.62494287
2	0	0	1	- 0.38494013
3	1	0	0	- 0.30571421 x 10^2
3	2	0	0	0.19808703 x 10^2
3	3	0	0	- 0.64883934 x 10^1
3	4	0	0	0.11339373 x 10^1
3	5	0	0	- 0.10044710
3	6	0	0	0.35361005 x 10^{-2}

Table 19 (Continued)

i	j	k	l	B_{ijkl}
3	0	1	0	0.77847012 x 10^{-2}
3	0	0	1	0.47599056 x 10^{-2}
0	1	1	0	- 0.76285305 x 10^2
0	1	0	1	0.28443009 x 10^2
0	2	1	0	0.45880414 x 10^2
0	2	0	1	- 0.15370153 x 10^2
0	3	1	0	- 0.14015423 x 10^2
0	3	0	1	0.42539016 x 10^1
0	4	1	0	0.23014694 x 10^1
0	4	0	1	- 0.63976158
0	5	1	0	- 0.19325122
0	5	0	1	0.50015047 x 10^{-1}
0	6	1	0	0.65059551 x 10^{-2}
0	6	0	1	- 0.15982473 x 10^{-2}
0	0	1	1	0.14194351
Correlation coefficient				0.9975
Standard deviation				0.2170

Table 20. Numerical values of B_{ijkl}'s for function $F^4(3d,3d)$ [eV]

i	j	k	l	B_{ijkl}
0	0	0	0	- 0.97738412 x 10^3
1	0	0	0	0.12131614 x 10^3
2	0	0	0	- 0.50935163 x 10^1
3	0	0	0	0.73143613 x 10^{-1}
0	1	0	0	0.16257306 x 10^3
0	2	0	0	- 0.78722443 x 10^2
0	3	0	0	0.83200777 x 10^1
0	0	1	0	0.59393664 x 10^2
0	0	0	1	- 0.53040154 x 10^1
1	1	0	0	- 0.13765830 x 10^2
1	2	0	0	0.73549267 x 10^1
1	3	0	0	- 0.84657804
1	0	1	0	- 0.81056878 x 10^1
1	0	0	1	- 0.15688674
2	1	0	0	0.35016806
2	2	0	0	- 0.21427645
2	3	0	0	0.27855185 x 10^{-1}
2	0	1	0	0.35763945
2	0	0	1	0.30463639 x 10^{-1}
3	1	0	0	- 0.26971048 x 10^{-2}
3	2	0	0	0.18940804 x 10^{-2}
3	3	0	0	- 0.29539367 x 10^{-3}
3	0	1	0	- 0.51809794 x 10^{-2}
3	0	0	1	- 0.66997175 x 10^{-3}
0	1	1	0	0.58955682

Table 20 (Continued)

i	j	k	l	B_{ijkl}
0	1	0	1	0.68601558
0	2	1	0	- 0.13967777
0	2	0	1	- 0.14433957
0	3	1	0	0.97608456 x 10^{-2}
0	3	0	1	0.78454603 x 10^{-2}
0	0	1	1	- 0.26415767 x 10^{-1}
Correlation coefficient				0.9906
Standard deviation				0.2550

Table 21. Numerical values of B_{ijk}'s for function $G^2(4s,3d)$ [eV]

i	j	k	B_{ijk}
0	0	0	- 0.11455318 x 10^4
1	0	0	0.92973076 x 10^2
2	0	0	- 0.17229575 x 10^1
0	1	0	0.25863178 x 10^4
0	2	0	- 0.19084621 x 10^4
0	3	0	0.62673258 x 10^3
0	4	0	- 0.82657276 x 10^2
0	5	0	- 0.10644581 x 10^1
0	6	0	0.11616411 x 10^1
0	7	0	- 0.71316415 x 10^{-1}
0	0	1	0.22219675 x 10^1
1	1	0	- 0.21820459 x 10^3
1	2	0	0.16768532 x 10^3
1	3	0	- 0.59443351 x 10^2
1	4	0	0.96717132 x 10^1
1	5	0	- 0.45948678
1	6	0	- 0.43470169 x 10^{-1}
1	7	0	0.39131452 x 10^{-2}
1	0	1	- 0.24871251 x 10^1
2	1	0	0.42410120 x 10^1
2	2	0	- 0.33535039 x 10^1
2	3	0	0.12424209 x 10^1
2	4	0	- 0.22181820
0	5	1	0.78248232
0	6	1	- 0.55145855 x 10^{-1}
0	7	1	0.15861732 x 10^{-2}
Correlation coefficient			0.9517
Standard deviation			0.1600

Table 22. Numerical values of B_{ijk}'s for function $G^1(4p,3d)$ [eV]

i	j	k	B_{ijk}
0	0	0	0.16555487 x 10^7
1	0	0	- 0.43654873 x 10^6
2	0	0	0.47957155 x 10^5
3	0	0	- 0.28087908 x 10^4
4	0	0	0.92485994 x 10^2
5	0	0	- 0.16230669 x 10^1
6	0	0	0.11858829 x 10^{-1}
0	1	0	- 0.31410610 x 10^5
0	2	0	0.17763564 x 10^6
0	3	0	- 0.28791767 x 10^5
0	0	1	0.11022272 x 10^6
1	1	0	0.51948525 x 10^4
1	2	0	- 0.39569733 x 10^5
1	3	0	0.66230471 x 10^4
1	0	1	- 0.26424377 x 10^5
2	1	0	- 0.40329310 x 10^3
2	2	0	0.36524915 x 10^4
2	3	0	- 0.63248152 x 10^3
2	0	1	0.26322274 x 10^4
3	1	0	0.22541847 x 10^2
3	2	0	- 0.17886380 x 10^3
3	3	0	0.32097795 x 10^2
3	0	1	- 0.13947191 x 10^3
4	1	0	- 0.95287396
4	2	0	0.49032886 x 10^1
4	3	0	- 0.91305851
4	0	1	0.41463954 x 10^1
5	1	0	0.24079772 x 10^{-1}
5	2	0	- 0.71402077 x 10^{-1}
5	3	0	0.13805248 x 10^{-1}
5	0	1	- 0.65584255 x 10^{-1}
6	1	0	- 0.25212255 x 10^{-3}
6	2	0	0.43206836 x 10^{-3}
6	3	0	- 0.86691202 x 10^{-4}
6	0	1	0.43122713 x 10^{-3}
0	1	1	- 0.98041671
0	2	1	0.20227796
0	3	1	- 0.11422109 x 10^{-1}
Correlation coefficient			0.9716
Standard deviation			0.1100

Table 23. Numerical values of B_{ijk}'s for function $F^2(4p,3d)$ [eV]

i	j	k	B_{ijk}
0	0	0	-0.42013352×10^2
1	0	0	-0.10733315×10^2
2	0	0	0.13420003×10^1
3	0	0	$-0.35139129 \times 10^{-1}$
0	1	0	0.38809453×10^3
0	2	0	-0.24670376×10^3
0	3	0	0.36228208×10^2
0	4	0	-0.26679394×10^1
0	0	1	-0.15030779×10^3
1	1	0	-0.43605595×10^2
1	2	0	0.31246634×10^2
1	3	0	-0.45599939×10^1
1	4	0	0.30507551
1	0	1	0.16949370×10^2
2	1	0	0.14636800×10^1
2	2	0	-0.13003577×10^1
2	3	0	0.19425625
2	4	0	$-0.12063524 \times 10^{-1}$
2	0	1	-0.62080669
3	1	0	$-0.12170482 \times 10^{-1}$
3	2	0	$0.17317047 \times 10^{-1}$
3	3	0	$-0.27233876 \times 10^{-2}$
3	4	0	$0.16160382 \times 10^{-3}$
3	0	1	$0.74668203 \times 10^{-2}$
0	1	1	-0.18199613×10^1
0	2	1	0.55839395
0	3	1	$-0.69845921 \times 10^{-1}$
0	4	1	$0.32721052 \times 10^{-2}$
Correlation coefficient			0.9765
Standard deviation			0.2411

Table 24. Numerical values of B_{ijk}'s for function $G^3(4p,3d)$ [eV]

i	j	k	B_{ijk}
0	0	0	0.10108317×10^3
1	0	0	-0.36844253×10^1
2	0	0	-0.23070281
0	1	1	-0.64177691×10^3
0	2	0	0.23328989×10^3
0	3	0	0.13705945×10^3
0	4	0	-0.11643706×10^3
0	5	0	0.30966279×10^2
0	6	0	-0.35575376×10^1

Table 24 (Continued)

i	j	k	B_{ijk}
0	7	0	0.15023608
0	0	1	-0.21189686×10^2
1	1	0	0.59326083×10^2
1	2	0	-0.35008750×10^2
1	3	0	0.46854902
1	4	0	0.53493135×10^1
1	5	0	-0.17523858×10^1
1	6	0	0.21798409
1	7	0	$-0.95967189 \times 10^{-2}$
1	0	1	0.39257747×10^1
2	1	0	-0.89742166
2	2	0	0.64833581
2	3	0	$-0.71816618 \times 10^{-1}$
2	4	0	$-0.68856443 \times 10^{-1}$
2	5	0	$0.26357942 \times 10^{-1}$
2	6	0	$-0.34623185 \times 10^{-2}$
2	7	0	$0.15691632 \times 10^{-3}$
2	0	1	$-0.73905081 \times 10^{-1}$
0	1	1	-0.64925936×10^2
0	2	1	0.54256204×10^2
0	3	1	-0.23079148×10^2
0	4	1	0.54686297×10^1
0	5	1	-0.73025711
0	6	1	$0.51319283 \times 10^{-1}$
0	7	1	$-0.14735746 \times 10^{-2}$
Correlation coefficient			0.9411
Standard deviation			0.2201

Resulting functions for $F^2(3d,3d)$ and $F^4(3d,3d)$ have the form of eqn (*18*), for $G^2(4s,3d)$, $G^1(4p,3d)$, $F^2(4p,3d)$, $G^3(4p,3d)$, $F^0(4s,3d)$, and $F^0(4p,3d)$ the form of eqn (*16*), for $G^1(4s,4p)$ the form of eqn (*15*), for $F^0(4s,4s)$ and $F^0(4s,4p)$ the form of eqn (*14*) and for $F^0(3d,3d)$ the form of eqn (*17*). Numerical values of coefficients B_{ijkl}, B_{ijk}, and B_{ij} are listed in Tables 13—24, where also the correlation coefficients of individual regression functions are included. Functional values of approximative expressions for electron configurations, available from spectral data, are listed in Tables 1—12 under the symbol Approximative. In these tables under the symbol Deviation the deviations of approximative values from experimental values of relevant integrals are also listed.

From the comparison of experimental and approximative values of individual Slater—Condon parameters it follows that suggested functions well agree with the dependence of spectral values on the electron configuration of an atom (ion). Therefore, we can use them for interpolation of the values relevant to noninteger electron configurations obtained by the population analysis in LCAO MO calculations. The analysis of the parameters $F^0(4p,4p)$, $F^2(4p,4p)$, $R^1(4s,3d,3d,3d)$, $R^1(4s,4p,4p,3d)$, and $R^2(4s,4p,4p,3d)$ which are necessary for enumeration of the monocentric repulsion integrals in the framework of LCAO MO approximation should be the content of the next paper of this series.

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Translated by M. Kozlik