Dependence of Slater—Condon parameters on electron configuration. III. Integrals $F^0(4p,4p)$, $F^2(4p,4p)$, $R^1(4s,3d,3d,3d)$, $R^1(4s,4p,4p,3d)$, and $R^2(4s,4p,4p,3d)$ for elements of the first transition series

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There is proposed a method of calculation of values of the integrals $F^0(4p,4p)$, $F^2(4p,4p)$, $R^1(4s,3d,3d,3d)$, $R^1(4s,4p,4p,3d)$, and $R^2(4s,4p,4p,3d)$ in dependence on electron configuration of atoms (ions) of the first transition series. The obtained values of individual integrals are consistent with values of other Slater—Condon parameters obtained by analysis of atomic spectra.

В работе предложен метод расчета величин интегралов $F^0(4p,4p)$, $F^2(4p,4p)$, $R^1(4s,3d,3d,3d)$, $R^1(4s,4p,4p,3d)$ и $R^2(4s,4p,4p,3d)$ в зависимости от электронной конфигурации атомов (ионов) первого переходного периода. Полученные величины отдельных интегралов консистентны с величинами параметров Слейтера—Кондона, полученными из анализа спектров атомов.

In the previous paper of this series [1] there were proposed regression functions for the dependence of Slater—Condon parameters (available from atomic spectroscopy data) on electron configuration of atoms (ions) of the first transition series.

The methods of quantum chemistry, which consider all the monocentric integrals of electron repulsion, require the knowledge of the Slater—Condon parameters $F^0(4p,4p)$ and $F^2(4p,4p)$, which cannot be determined because of the lack of experimental data for elements of the first transition series. There is also necessary [2] to know the values of the integrals $R^1(4s,3d,3d,3d)$, $R^1(4s,4p,4p,3d)$, and

$R^2(4s,4p,4p,3d)$ which do not belong to 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. In this work there is suggested a procedure of calculation of such parameters in dependence on electron configuration of atoms (ions), which is consistent with analogous dependences proposed for other spectral available parameters [1].

Method and results

Theoretical values of the integrals $F^0(4p,4p)$, $F^2(4p,4p)$, $R^1(4s,3d,3d,3d)$, $R^1(4s,4p,4p,3d)$, and $R^2(4s,4p,4p,3d)$ can be calculated by direct integration, using a particular type of atomic orbitals. The use of theoretical values of these integrals, however, would not be consistent with the use of empirical values of the other integrals. Moreover, theoretical values of these integrals are dependent on the basis of atomic orbitals, used for integration. We have tried to overcome these difficulties introducing the assumption that the ratio of theoretical values of two different types of integrals is approximatively the same as this quantity determined by analysis of atomic spectra

$$\left(\frac{\text{Integral}_A}{\text{Integral}_B}\right)_{\text{theor}} = \left(\frac{\text{Integral}_A}{\text{Integral}_B}\right)_{\text{exp}} \tag{1}$$

The validity of this relation was tested for some cases of pairs of Slater—Condon parameters for elements of the first transition series. Only such pairs of Slater—Condon parameters were considered, in which at least one equal atomic orbital occurs. Theoretical values were calculated using the basis of atomic orbitals of *Richardson et al.* [3, 4]. In this basis there were calculated the values of the Slater—Condon parameters $G^1(4s,4p)$ and $F^2(4p,4p)$ and the ratio of the theoretical values was obtained

$$\left(\frac{G^1(4s,4p)}{F^2(4p,4p}\right)_{\text{theor}}$$

This ratio depends only on the charge of the atom and is independent of the atomic number. Therefore, this ratio was approximated as continuous function of the atomic charge

$$\left(\frac{G^1(4s,4p)}{F^2(4p,4p)}\right)_{\text{theor}} = \sum_{i=0}^{2} B_i Q^i \tag{2}$$

In Table 15 there are listed the values of coefficients B_i and the correlation coefficient of this approximation. The values of the parameter $F^2(4p,4p)$ we

Table 1. Theoretical and calculated values of the ratio $F^0(4p,4p)/F^0(4s,4p)$ [eV]

Z	Q	Theoretical	Calculated	Deviation
22	0	0.8550	0.8566	-0.0016
22	1	0.9532	0.9513	0.0018
22	2	1.0406	1.0461	-0.0055
23	0	0.8501	0.8512	-0.0011
23	1	0.9550	0.9523	0.0026
23	2	1.0550	1.0535	0.0016
24	0	0.8469	0.8471	-0.0002
24	1	0.9566	0.9526	0.0039
24	2	1.0647	1.0582	0.0065
25	0	0.8441	0.8441	0.0000
25	1	0.9517	0.9522	-0.0005
25	2	1.0591	1.0604	-0.0013
26	0	0.8408	0.8424	-0.0015
26	1	0.9504	0.9512	-0.0008
26	2	1.0538	1.0599	-0.0061
27	0	0.8410	0.8418	-0.0008
27	1	0.9520	0.9494	0.0026
27	2	1.0523	1.0569	-0.0046
28	0	0.8411	0.8425	-0.0014
28	1	0.9505	0.9469	0.0036
28	2	1.0540	1.0513	0.0027

Table 2. Theoretical and calculated values of the ratio $F^0(4p,4p)/F^0(4p,3d)$ [eV]

Z	Q	Theoretical	Calculated	Deviation
22	0	0.8114	0.8102	0.0012
22	1	0.8187	0.8168	0.0019
22	2	0.8165	0.8165	0.0000
23	0	0.8088	0.8094	-0.0006
23	1	0.8148	0.8155	-0.0007
23	2	0.8169	0.8153	0.0016
24	0	0.8082	0.8085	-0.0003
24	1	0.8142	0.8143	-0.0001
24	2	0.8138	0.8141	-0.0003
25	0	0.8069	0.8077	-0.0007
25	1	0.8103	0.8130	-0.0028
25	2	0.8126	0.8129	-0.0004
26	0	0.8064	0.8068	-0.0005
26	1	0.8120	0.8118	0.0002
26	2	0.8086	0.8117	-0.0031
27	0	0.8063	0.8060	0.0003
27	1	0.8108	0.8105	0.0003
27	2	0.8120	0.8105	0.0014
28	0	0.8058	0.8051	0.0006
28	1	0.8105	0.8093	0.0012
28	2	0.8103	0.8093	0.0009

Table 3. Theoretical and calculated values of the ratio $G^1(4s,4p)/F^2(4p,4p)$ [eV]

Q	Theoretical	Calculated	Deviation
0	0.9421	0.9421	0.0000
1	1.3255	1.3255	0.0000
2	1.2001	1.2001	0.0000

Table 4. Theoretical and calculated values of the ratio $R^1(4s,4p,4p,3d)/$ $/G^3(4p,3d)$ [eV]

Z	Q	Theoretical	Calculated	Deviation
22	0	2.9748	3.0050	-0.0302
22	1	2.5452	2.5470	-0.0017
22	2	2.1589	2.1011	0.0578
23	0	3.2717	3.2776	-0.0059
23	1	2.6483	2.6583	0.0100
23	2	2.1410	2.1527	-0.0116
24	0	3.5556	3.5503	0.0053
24	1	2.7507	2.7696	-0.0189
24	2	2.1379	2.2043	-0.0664
25	0	3.8418	3.8229	0.0188
25	1	2.9008	2.8808	0.0200
25	2	2.2303	2.2559	-0.0255
26	0	4.1561	4.0955	0.0605
26	1	3.0222	2.9921	0.0301
26	2	2.3169	2.3074	0.0094
27	0	4.3802	4.3681	0.0121
27	1	3.1036	3.1034	0.0002
27	2	2.3883	2.3590	0.0293
28	0	4.5802	4.6408	-0.0606
28	1	3.2105	3.2147	-0.0419
28	2	2.4233	2.4106	0.0127
29	1	3.3105	3.3260	-0.0159
29	2	2.4565	2.4622	-0.0057

Table 5. Theoretical and calculated values of the ratio $R^2(4s,4p,4p,3d)/$ $/G^1(4p,3d)$ [eV]

Z	Q	Theoretical	Calculated	Deviation
22	0	1.5212	1.5322	-0.0110
22	1	1.4435	1.4500	-0.0065
22	2	1.3792	1.3554	0.0239
23	0	1.6607	1.6663	-0.0056
23	1	1.5082	1.5138	-0.0057

Table 5 (Continued)

Z	Q	Theore-tical	Calcu-lated	Devia-tion
23	2	1.3827	1.3876	-0.0049
24	0	1.8018	1.8003	0.0015
24	1	1.5718	1.5776	-0.0059
24	2	1.3879	1.4198	-0.0319
25	0	1.9430	1.9344	0.0086
25	1	1.6548	1.6415	0.0133
25	2	1.4422	1.4520	-0.0099
26	0	2.0960	2.0684	0.0276
26	1	1.7229	1.7053	0.0176
26	2	1.4910	1.4843	0.0067
27	0	2.2092	2.2025	0.0067
27	1	1.7718	1.7691	0.0027
27	2	1.5341	1.5165	0.0176
28	0	2.3087	2.3366	-0.0278
28	1	1.8302	1.8329	-0.0027
28	2	1.5550	1.5487	0.0063
29	1	1.8838	1.8967	-0.0129
29	2	1.5732	1.5809	-0.0077

Table 6. Theoretical and calculated values of the ratio $R^2(4s,4p,4p,3d)/F^2(4p,3d)$ [eV]

Z	Q	Theore-tical	Calcu-lated	Devia-tion
22	0	0.8427	0.8404	0.0023
22	1	0.8639	0.8656	-0.0017
22	2	0.7137	0.7037	0.0100
23	0	0.8280	0.8270	0.0010
23	1	0.8602	0.8608	-0.0006
23	2	0.6975	0.6989	-0.0014
24	0	0.8148	0.8136	0.0012
24	1	0.8565	0.8560	0.0005
24	2	0.6839	0.6941	-0.0102
25	0	0.7990	0.8002	-0.0013
25	1	0.8526	0.8513	0.0013
25	2	0.6848	0.6892	-0.0044
26	0	0.7771	0.7868	-0.0097
26	1	0.8490	0.8465	0.0025
26	2	0.6842	0.6844	-0.0002
27	0	0.7731	0.7734	-0.0003
27	1	0.8421	0.8417	0.0004
27	2	0.6827	0.6796	0.0031
28	0	0.7669	0.7600	0.0069
28	1	0.8365	0.8370	-0.0005
28	2	0.6764	0.6747	0.0017
29	1	0.8303	0.8322	-0.0019
29	2	0.6714	0.6699	0.0015

Table 7. Theoretical and calculated values of the ratio $R^2(4s,4p,4p,3d)/G^2(4s,3d)$ [eV]

Z	Q	Theore-tical	Calcu-lated	Devia-tion
22	0	0.4793	0.4633	0.0160
22	1	1.2182	1.2432	-0.0249
22	2	1.8341	1.9056	-0.0716
23	0	0.4475	0.4479	-0.0004
23	1	1.2809	1.2797	0.0012
23	2	1.9902	1.9791	0.0111
24	0	0.4273	0.4325	-0.0053
24	1	1.3431	1.3161	0.0270
24	2	2.1121	2.0525	0.0596
25	0	0.4073	0.4171	-0.0098
25	1	1.3556	1.3526	0.0030
25	2	2.1639	2.1260	0.0379
26	0	0.3799	0.4017	-0.0022
26	1	1.3877	1.3891	-0.0014
26	2	2.2021	2.1994	0.0027
27	0	0.3867	0.3863	0.0004
27	1	1.4381	1.4256	0.0125
27	2	2.2669	2.2728	-0.0059
28	0	0.3919	0.3709	0.0209
28	1	1.4616	1.4621	-0.0005
28	2	2.3346	2.3463	-0.0116
29	1	1.4816	1.4985	0.0169
29	2	2.3975	2.4197	-0.0222

Table 8. Theoretical and calculated values of the ratio $R^2(4s,3d,3d,3d)/G^2(4s,3d)$ [eV]

Z	Q	Theore-tical	Calcu-lated	Devia-tion
22	0	0.9745	0.9749	-0.0004
22	1	0.9574	0.9442	0.0133
22	2	0.8036	0.7714	0.0322
23	0	0.9420	0.9387	0.0034
23	1	0.8936	0.8891	0.0045
23	2	0.6932	0.6961	-0.0029
24	0	0.9029	0.9024	0.0004
24	1	0.8284	0.8340	-0.0056
24	2	0.6078	0.6207	-0.0130
25	0	0.8650	0.8662	-0.0012
25	1	0.7673	0.7789	-0.0116
25	2	0.5267	0.5454	-0.0187
26	0	0.8255	0.8299	-0.0045
26	1	0.7128	0.7238	-0.0110
26	2	0.4560	0.4700	-0.0140
27	0	0.7904	0.7937	-0.0033

Table 8 (Continued)

Z	Q	Theoretical	Calculated	Deviation
27	1	0.6617	0.6687	-0.0070
27	2	0.3816	0.3947	-0.0131
28	0	0.7631	0.7574	0.0056
28	1	0.6151	0.6136	0.0015
28	2	0.3196	0.3193	0.0003
29	1	0.5745	0.5585	0.0160
29	2	0.2733	0.2440	0.0293

Table 9. Theoretical and calculated values of the ratio $R^2(4s,4p,4p,3d)/$ $/G^2(4p,3d)$ [eV]

Z	Q	Theoretical	Calculated	Deviation
22	0	2.3044	2.3276	-0.0230
22	1	2.0037	2.0076	-0.0039
22	2	1.7386	1.6975	0.0411
23	0	2.5220	2.5276	-0.0055
23	1	2.0821	2.0898	-0.0078
23	2	1.7269	1.7354	-0.0084
24	0	2.7324	2.7228	0.0049
24	1	2.1595	2.1721	-0.0126
24	2	1.7243	1.7732	-0.0489
25	0	2.9431	2.9275	0.0156
25	1	2.2710	2.2544	0.0166
25	2	1.7932	1.8110	-0.0178
26	0	3.1734	3.1275	0.0459
26	1	2.3606	2.3367	0.0239
26	2	1.8566	1.8488	0.0078
27	0	3.3367	3.3275	0.0092
27	1	2.4202	2.4189	0.0013
27	2	1.9095	1.8866	0.0228
28	0	3.4807	3.5274	-0.0468
28	1	2.4977	2.5012	-0.0035
28	2	1.9339	1.9244	0.0094
29	1	2.5695	2.5835	-0.0140
29	2	1.9562	1.9623	-0.0061

Table 10. Theoretical and calculated values of the ratio $R^1(4s,4p,4p,3d)/$ $/F^2(4p,3d)$ [eV]

Z	Q	Theoretical	Calculated	Deviation
22	0	1.0879	1.0864	0.0015
22	1	1.0974	1.0989	-0.0015

Table 10 (Continued)

Z	Q	Theoretical	Calculated	Deviation
22	2	0.8862	0.8715	0.0148
23	0	1.0741	1.0722	0.0019
23	1	1.0941	1.0950	-0.0009
23	2	0.8648	0.8671	-0.0023
24	0	1.0603	1.0580	0.0022
24	1	1.0910	1.0912	-0.0002
24	2	0.8479	0.8627	-0.0148
25	0	1.0429	1.0438	-0.0009
25	1	1.0890	1.0874	0.0017
25	2	0.8517	0.8583	-0.0066
26	0	1.0178	1.0297	-0.0119
26	1	1.0870	1.0835	0.0035
26	2	0.8539	0.8539	0.0000
27	0	1.0148	1.0155	-0.0007
27	1	1.0799	1.0797	0.0003
27	2	0.8539	0.8495	0.0043
28	0	1.0009	1.0013	0.0079
28	1	1.0752	1.0758	-0.0006
28	2	0.8476	0.8452	0.0024
29	1	1.0698	1.0720	-0.0022
29	2	0.8430	0.8408	0.0022

Table 11. Theoretical and calculated values of the ratio $R^1(4s,4p,4p,3d)/$ $/G^1(4p,3d)$ [eV]

Z	Q	Theoretical	Calculated	Deviation
22	0	1.9637	1.9780	-0.0143
22	1	1.8336	1.8395	-0.0059
22	2	1.7126	1.6776	0.0350
23	0	2.1544	2.1607	-0.0063
23	1	1.9183	1.9256	-0.0072
23	2	1.7142	1.7213	-0.0071
24	0	2.3447	2.3434	0.0013
24	1	2.0020	2.0116	-0.0096
24	2	1.7208	1.7650	-0.0442
25	0	2.5363	2.5260	0.0102
25	1	2.1137	2.0976	0.0161
25	2	1.7937	1.8087	-0.0150
26	0	2.7451	2.7087	0.0364
26	1	2.2059	2.1837	0.0222
26	2	1.8606	1.8524	0.0082
27	0	2.9001	2.8914	0.0087
27	1	2.2721	2.2697	0.0024
27	2	1.9188	1.8962	0.0226
28	0	3.0381	3.0341	-0.0360
28	1	2.3525	2.3558	-0.0033

Table 11 (Continued)

Z	Q	Theoretical	Calculated	Deviation
28	2	1.9486	1.9399	0.0087
29	1	2.4271	2.4418	-0.0147
29	2	1.9754	1.9835	-0.0082

Table 12. Theoretical and calculated values of the ratio $R^1(4s,4p,4p,3d)/G^2(4s,3d)$ [eV]

Z	Q	Theoretical	Calculated	Deviation
22	0	0.6187	0.5990	0.0197
22	1	1.5475	1.5775	-0.0300
22	2	2.2774	2.3581	-0.0807
23	0	0.5805	0.5807	-0.0001
23	1	1.6292	1.6278	0.0014
23	2	2.4674	2.4549	0.0126
24	0	0.5560	0.5623	-0.0063
24	1	1.7108	1.6780	0.0328
24	2	2.6187	2.5516	0.0671
25	0	0.5317	0.5440	-0.0123
25	1	1.7315	1.7283	0.0032
25	2	2.6914	2.6484	0.0430
26	0	0.4976	0.5257	-0.0281
26	1	1.7767	1.7786	-0.0018
26	2	2.7480	2.7452	0.0028
27	0	0.5077	0.5073	0.0004
27	1	1.8441	1.8288	0.0153
27	2	2.8354	2.8419	-0.0065
28	0	0.5156	0.4890	0.0267
28	1	1.8787	1.8791	-0.0004
28	2	2.9255	2.9387	-0.0132
29	1	1.9090	1.9294	-0.0204
29	2	3.0105	3.0355	-0.0250

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

i	j	B_{ij}
0	0	1.2786674
1	0	$-3.2422538 \times 10^{-2}$
2	0	6.0161706×10^{-4}
0	1	$-5.2572886 \times 10^{-1}$
1	1	4.9107077×10^{-2}
2	1	$-9.5010119 \times 10^{-4}$

Table 13 (Continued)

Correlation coefficient	0.999355
Standard deviation	0.0036

Table 14. Numerical values of B_{ij}'s for the ratio $F^0(4p,4p)/F^0(4p,3d)$ [eV]

i	j	B_{ij}
0	0	8.2899525×10^{-1}
1	0	$-8.5282143 \times 10^{-4}$
0	1	2.3566518×10^{-2}
0	2	$-8.2801607 \times 10^{-3}$
1	1	$-6.1866071 \times 10^{-4}$
1	2	2.2187500×10^{-4}
Correlation coefficient		0.938731
Standard deviation		0.0015

Table 15. Numerical values of B_i's for the ratio $G^1(4s,4p)/F^2(4p,4p)$ [eV]

i	B_i
0	9.420520×10^{-1}
1	6.377890×10^{-1}
2	-2.543860×10^{-1}
Correlation coefficient	0.999999
Standard deviation	0.0000

Table 16. Numerical values of B_{ij}'s for the ratio $R^1(4s,4p,4p,3d)/G^3(4p,3d)$ [eV]

i	j	B_{ij}
0	0	-2.9929301
1	0	2.7263382×10^{-1}
0	1	4.2032872
0	2	-1.1118345
1	1	$-2.1215568 \times 10^{-1}$
1	2	5.0814881×10^{-2}
Correlation coefficient		0.999118
Standard deviation		0.0347

estimate using relation (*2*), where for $G^1(4s,4p)$ we place the values of approximative function for experimental values of this parameter (see Ref. [1]).

Analogous procedure was used for estimation of values of the parameter $F^0(4p,4p)$. The ratios

$$\left(\frac{F^0(4p,4p)}{F^0(4s,4p)}\right)_{\text{theor}} \quad \text{and} \quad \left(\frac{F^0(4p,4p)}{F^0(4p,3d)}\right)_{\text{theor}}$$

were calculated for various atoms of the first transition series in the basis of *Richardson*'s orbitals [3, 4]. These ratios were approximated by continuous functions of atomic number and atomic charge

$$\left(\frac{F^0(4p,4p)}{F^0(4s,4p)}\right)_{\text{theor}} = \sum_{i=0}^{2}\sum_{j=0}^{1} B_{ij}Z^iQ^j \tag{3}$$

$$\left(\frac{F^0(4p,4p)}{F^0(4p,3d)}\right)_{\text{theor}} = \sum_{i=0}^{1}\sum_{j=0}^{2} B_{ij}Z^iQ^j \tag{4}$$

The coefficients B_{ij} are listed in Tables 13 and 14. The numerical values of $F^0(4p,4p)$ we obtain as the arithmetic mean of values obtained by both methods using relations (*3*) and (*4*), when we replace $F^0(4s,4p)$ and $F^0(4p,3d)$ by values obtained from approximative functions introduced in the previous paper of this series [1]. The use of the arithmetic mean for calculation of $F^0(4p,4p)$ compensates errors originated in approximative character of the used function relations.

Values of the integrals $R^1(4s,3d,3d,3d)$, $R^1(4s,4p,4p,3d)$, and $R^2(4s,4p,4p,3d)$ consistent with spectral values of the other integrals were for elements of the first transition series obtained by analogous procedure as the Slater—Condon parameters $F^0(4p,4p)$ and $F^2(4p,4p)$. For the ratios of theoretically calculated integrals in the basis of *Richardson*'s atomic orbitals [3, 4] there were used functions of the type

$$F(Z,Q) = \sum_{i=0}^{N_Z}\sum_{j=0}^{N_Q} B_{ij}Z^iQ^j \tag{5}$$

where Z is the atomic number, Q is the charge of the atom, N_Z and N_Q are the optimum degrees of polynomials, obtained by maximization of the correlation coefficient. In Tables 16—24 there are listed coefficients B_{ij} of these functions, obtained by the least-squares method. Values of the R integrals are calculated as the arithmetic mean of all the approximations containing competent atomic orbitals.

In Tables 1—12 are under the symbol Theoretical listed values of the ratios of individual types of integrals, obtained as a result of the direct integration and under the symbol Calculated values obtained by approximative expressions. From the

Table 17. Numerical values of B_{ij_1}'s for the ratio $R^2(4s,4p,4p,3d)/G^1(4p,3d)$ [eV]

i	j	B_{ij}
0	0	-1.4172170
1	0	1.3406389 x 10^{-1}
0	1	1.8947414
0	2	-4.3145859 x 10^{-1}
1	1	-8.9576363 x 10^{-2}
1	2	1.9328268 x 10^{-2}
Correlation coefficient		0.998451
Standard deviation		0.0167

Table 18. Numerical values of B_{ij_2}'s for the ratio $R^2(4s,4p,4p,3d)/F^2(4p,3d)$ [eV]

i	j	B_{ij}
0	0	1.1350524
1	0	-1.3393286 x 10^{-2}
0	1	-1.6705907 x 10^{-1}
0	2	2.2942500 x 10^{-3}
1	1	1.2985940 x 10^{-2}
1	2	-4.3533452 x 10^{-3}
Correlation coefficient		0.998269
Standard deviation		0.0049

Table 19. Numerical values of B_{ij_2}'s for the ratio $R^2(4s,4p,4p,3d)/G^2(4s,3d)$ [eV]

i	j	B_{ij}
0	0	8.0207486 x 10^{-1}
1	0	-1.5397571 x 10^{-2}
0	1	-4.6683375 x 10^{-1}
0	2	1.0540021 x 10^{-1}
1	1	5.9335280 x 10^{-2}
1	2	-7.4587798 x 10^{-3}
Correlation coefficient		0.999401
Standard deviation		0.0287

Table 20. Numerical values of B_{ij_2}'s for the ratio $R^2(4s,3d,3d,3d)/G^2(4s,3d)$ [eV]

i	j	B_{ij}
0	0	1.7722911
1	0	-3.6244357 x 10^{-2}
0	1	4.3937877 x 10^{-1}
0	2	-5.5474875 x 10^{-2}
1	1	-1.8141464 x 10^{-2}
1	2	-7.0580952 x 10^{-4}
Correlation coefficient		0.998004
Standard deviation		0.0147

Table 21. Numerical values of B_{ij_3}'s for the ratio $R^2(4s,4p,4p,3d)/G^3(4p,3d)$ [eV]

i	j	B_{ij}
0	0	-2.0716638
1	0	1.9996736 x 10^{-1}
0	1	3.0700209
0	2	-8.0070159 x 10^{-1}
1	1	-1.5432089 x 10^{-1}
1	2	3.6622833 x 10^{-2}
Correlation coefficient		0.999023
Standard deviation		0.0262

Table 22. Numerical values of B_{ij_2}'s for the ratio $R^1(4s,4p,4p,3d)/F^2(4p,3d)$ [eV]

i	j	B_{ij}
0	0	1.3985521
1	0	-1.4188000 x 10^{-2}
0	1	-2.1509982 x 10^{-1}
0	2	-1.0796429 x 10^{-4}
1	1	1.5794690 x 10^{-2}
1	2	-5.4463810 x 10^{-3}
Correlation coefficient		0.998453
Standard deviation		0.0067

Table 23. Numerical values of B_{ij_1}'s for the ratio $R^1(4s,4p,4p,3d)/G^1(4p,3d)$ [eV]

i	j	B_{ij}
0	0	-2.0408394
1	0	1.8267550×10^{-1}
0	1	-2.5965878
0	2	$-6.0914262 \times 10^{-1}$
1	1	$-1.2378893 \times 10^{-1}$
1	2	2.7155196×10^{-2}
Correlation coefficient		0.998665
Standard deviation		0.0222

Table 24. Numerical values of B_{ij_2}'s for the ratio $R^1(4s,4p,4p,3d)/G^2(4s,3d)$ [eV]

i	j	B_{ij}
0	0	1.0022841
1	0	$-1.8331857 \times 10^{-2}$
0	1	$-6.7482857 \times 10^{-1}$
0	2	1.4412793×10^{-1}
1	1	7.9651060×10^{-2}
1	2	$-1.1049952 \times 10^{-2}$
Correlation coefficient		0.999479
Standard deviation		0.0331

magnitude of deviations we can conclude that the proposed regression functions are in a very good agreement with the theoretical values of the ratios of individual integrals.

In connection with the results shown in [1] we can enumerate values of all the monocentric integrals of electron repulsion for atoms of the first transition series for noninteger electron configurations obtained by population analysis in LCAO MO SCF methods.

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