Inner-Shell Excitation Energies for C-, N-, O-, and F-like Ions with Z = 6 - 54

U. I. Safronova and A.S.Shlyaptseva
Department of Physics, University of Nevada, Reno
Reno, NV 89557

1 Introduction

In this paper we continue to study the atomic characteristics for doubly-excited states. In our previous paper [1] we developed a method for the calculation of energies for systems with three, four and five electrons such as $1s2s^n2p^{n'}$ ($n+n'$=2-4). This method was based on a perturbation theory starting with nonrelativistic hydrogenic basis functions. Moreover, the diagram technique was used. We treated these systems as states with an empty core and three, four and five electrons interacting with the nucleus and with each other. For such states only diagrams without loops give contributions to the nonrelativistic part of the energy. Here we study $1s2s^n2p^{n'}$ ($n+n'$=5, 6, 7, 8) states. Following the same approach, we must consider the states with an empty core and 6, 7, 8 and 9 electrons interacting with the nucleus and with each other. Obviously, it is more convenient to use hole representation, which allows to consider these states as systems with $8-n-n'$ holes and a non-empty core with two closed shells. In this approach we can treat these systems as states with a $1s^22s^22p^6$ core and 4, 3, 2 and 1 electrons interacting with the nucleus, the core and with each other. To describe the interaction of electrons with the core we have to take into account also diagrams with loops. For singly-excited states, these diagrams were studied in detail for systems with one electron above the core in many papers by Johnson et al (see, for example, [2]), and with two and three electrons above the core in papers [3, 4]. In these papers [2, 3, 4] relativistic basis functions were used, and all angular reductions for diagram contributions were given using the jj-coupling scheme. For two electrons above the core, the LS-coupling scheme was implemented in the paper by Safronova et al [5]. The first study of doubly-excited states using perturbation theory with including the first and second order diagram contributions (relevant to nonrelativistic energy) was presented in papers [6, 7].

2 Energies of $1s2s^n2p^{n'}$ States with $n+n'$=5, 6, 7, 8 in the Hole Representation

The field formulation of perturbation theory allows to construct the function of the n-hole system similar to the function of a n-electron system, replacing an operator of creation $a^+_{\beta_k}$ with an operator of annihilation a_{β_k}:

$$\Phi_n^Q = \frac{1}{n!}\sum_{\beta_1...\beta_n} C^Q_{\beta_1...\beta_n} a_{\beta_1}...a_{\beta_n}\Phi_0 \qquad (1)$$

Here Φ_0 and Q relate to the core and an atomic system with quantum numbers L, S, M, M$_S$, respectively. Index β_i describes a one-hole system with quantum numbers $n_il_im_im_{S_i}$, and $C^Q_{\beta_1...\beta_n}$

coefficients provide the antisymmetry in all indexes of the wave function Φ_n^Q (for detail see [5]). Using this determination of a hole-function we can carry out all calculations of diagram contributions. The functions of doubly-excited states $1s2s^n2p^{n'}[LSJ]$ with $n+n'$=5, 6, 7, 8 are written as follows

$$\begin{array}{rr}\Phi_1^Q=\frac{1}{1!}\sum_{\beta_1}C^Q_{\beta_1}a_{\beta_1}\Phi_0, & \Phi_2^Q=\frac{1}{2!}\sum_{\beta_1\beta_2}C^Q_{\beta_1\beta_2}a_{\beta_1}a_{\beta_2}\Phi_0,\\ \Phi_3^Q=\frac{1}{3!}\sum_{\beta_1\beta_2\beta_3}C^Q_{\beta_1\beta_2\beta_3}a_{\beta_1}a_{\beta_2}a_{\beta_3}\Phi_0, & \Phi_4^Q=\frac{1}{4!}\sum_{\beta_1\beta_2\beta_3\beta_4}C^Q_{\beta_1\beta_2\beta_3\beta_4}a_{\beta_1}a_{\beta_2}a_{\beta_3}a_{\beta_4}\Phi_0\end{array} \qquad (2)$$

The nl quantum numbers for Φ_1^Q, Φ_2^Q, Φ_3^Q and Φ_1^Q should be equal to $1s$, $1s2l$, $1s2l2l'$ and $1s2l2l'2l''$ accordingly. Briefly, we can represent our states as

$$\begin{array}{c}1s2s^22p^6\rightarrow 1s^{-1}\Phi_0,\\ 1s2s^22p^5\rightarrow 1s^{-1}2p^{-1}\Phi_0, 1s2s2p^6\rightarrow 1s^{-1}2s^{-1}\Phi_0,\\ 1s2s^22p^4\rightarrow 1s^{-1}2p^{-2}\Phi_0, 1s2s2p^5\rightarrow 1s^{-1}2s^{-1}2p^{-1}\Phi_0, 1s2p^6\rightarrow 1s^{-1}2s^{-2}\Phi_0,\\ 1s2s^22p^3\rightarrow 1s^{-1}2p^{-3}\Phi_0, 1s2s2p^4\rightarrow 1s^{-1}2s^{-1}2p^{-2}\Phi_0, 1s2p^3\rightarrow 1s^{-1}2s^{-2}2p^{-1}\Phi_0.\end{array} \qquad (3)$$

3 Results and Discussions

Tables 1,2,3 illustrate our results of calculations of the energies of N-, O- and F-like ions, respectively. The intermediate LS energies are shown only in the case of two identical terms belonging to one complex (the states with one parity and the same J but different QLS), for example, for $1s2s2p^n$ with n=4, 5 (^3P terms for C-like ions; ^2P terms for N-like ions). The same inter-electron interactions mix terms belonging to different configurations: $1s2s^22p^n+1s2p^{n+2}$ (^3P, ^1P terms for n= 4 and ^2S term for n= 5) and $1s^22s^22p^n+1s^22p^{n+2}$ (^1S, ^1D, ^3P terms for n= 4, ^2P term for n= 5 and ^1S term for n= 5). This mixing can be described by a first order perturbation theory diagram for the correlation part of the energy [5] and can be calculated by any computer method. The next part of the correlation energy can be obtained by using virtual configurations, both discrete and continuous. The advantage of the MZ program is to take into account this part of the correlation energy in the framework of second order perturbation theory. As a result, we believe that data obtained by this method for 2 - 10 electron systems are more precise than other methods.

We conclude that the absolute energy data given in Tables 1 - 3 can be used for many applications, particuarly in electron and photon emission spectroscopy.

References

[1] U. I. Safronova and A. S. Shlyaptseva, *Physica Scripta* **54**, 254 (1996)

[2] W. R. Johnson, M. Idrees, and J. Sapirstein, *Phys. Rev. A* **35**, 3218 (1987)

[3] M. S. Safronova, W. R. Johnson, and U. I. Safronova, *Phys. Rev. A***53**, 4036 (1996)

[4] M. S. Safronova, W. R. Johnson, and U. I. Safronova, *Phys. Rev. A* **54**, 2850 (1996)

[5] M. S. Safronova, U. I. Safronova, N. Nakamura, and S. Ohtani, *Physica Scripta* **53**, 689 (1996)

[6] U. I. Safronova and V. N. Kharitonova, *Optic and Spectroscopy* **27**, 550 (1969)

[7] U. I. Safronova, A. N. Ivanova, N. V. Rabinkina, and V. N. Kharitonova, *Optic and Spectroscopy* **28**, 841 (1970)

Table 1: Absolute values of the energy (E in $10^4 cm^{-1}$) for N-like systems. Designations: E=$1s^22s^22p^3$, F=$1s^22p^5$, C=$1s^22s2p^4$, I=$1s2s^22p^4$, J=$1s2p^6$, Q=$2s2p^5[^1P]1s$, K=$2s2p^5[^3P]1s$

N	LSJ	$Z = 12$	$Z = 14$	$Z = 16$	$Z = 18$	$Z = 20$	$Z = 22$	$Z = 24$	$Z = 26$
E	$^4S_{3/2}$	4111.650	5778.113	7737.435	9984.808	12523.56	15355.35	18482.17	21906.01
E	$^2D_{3/2}$	4106.136	5771.217	7729.207	9975.336	12512.96	15343.73	18469.54	21892.12
E	$^2D_{5/2}$	4106.137	5771.190	7729.087	9974.994	12512.19	15342.26	18467.07	21888.39
E	$^2P_{1/2}$	4103.307	5767.632	7724.794	9969.953	12506.38	15335.66	18459.65	21880.12
E	$^2P_{3/2}$	4103.297	5767.577	7724.608	9969.462	12505.28	15333.52	18455.87	21873.95
C	$^4P_{1/2}$	4086.832	5746.795	7699.505	9940.093	12471.81	15296.22	18415.18	21828.46
C	$^4P_{3/2}$	4086.659	5746.424	7698.798	9938.859	12469.79	15293.08	18410.50	21821.73
C	$^4P_{5/2}$	4086.567	5746.230	7698.439	9938.258	12468.87	15291.76	18408.74	21819.55
C	$^2D_{3/2}$	4077.487	5735.064	7685.314	9923.337	12452.34	15273.86	18389.68	21801.54
C	$^2D_{5/2}$	4077.490	5735.062	7685.295	9923.266	12452.15	15273.43	18388.83	21799.87
C	$^2S_{1/2}$	4071.480	5727.631	7676.482	9913.147	12440.85	15261.09	18375.65	21786.14
C	$^2P_{1/2}$	4069.223	5725.140	7673.769	9910.201	12437.62	15257.52	18371.62	21781.53
C	$^2P_{3/2}$	4069.019	5724.687	7672.873	9908.574	12434.87	15253.13	18364.97	21771.88
F	$^2P_{1/2}$	4046.439	5695.997	7638.127	9867.868	12388.37	15201.08	18307.71	21709.88
F	$^2P_{3/2}$	4046.170	5695.411	7637.003	9865.900	12385.15	15196.09	18300.32	21698.21
I	$^2S_{1/2}$	3071.879	4335.644	5825.308	7535.612	9469.301	11627.34	14010.93	16621.10
I	$^2P_{1/2}$	3074.837	4339.087	5829.303	7540.382	9475.299	11635.28	14021.71	16635.77
I	$^2P_{3/2}$	3075.046	4339.475	5829.901	7541.141	9476.049	11635.73	14021.52	16634.63
I	$^4P_{1/2}$	3082.650	4348.944	5841.125	7554.032	9490.582	11651.98	14039.72	16655.21
I	$^4P_{3/2}$	3082.763	4349.172	5841.529	7554.678	9491.529	11653.27	14041.34	16657.11
I	$^4P_{5/2}$	3083.028	4349.705	5842.496	7556.308	9494.115	11657.17	14046.97	16664.89
I	$^2D_{3/2}$	3076.258	4341.136	5832.071	7543.975	9479.830	11640.86	14028.50	16643.94
I	$^2D_{5/2}$	3076.328	4341.222	5832.121	7543.869	9479.355	11639.72	14026.31	16640.33
J	$^2S_{1/2}$	3018.043	4268.472	5744.511	7440.884	9360.351	11503.91	13872.78	16468.02
Q	$^2P_{1/2}$	3039.916	4296.820	5779.363	7482.305	9408.425	11558.72	13934.39	16536.46
Q	$^2P_{3/2}$	3040.060	4297.113	5779.906	7483.251	9409.990	11561.20	13938.15	16541.95
K	$^2P_{1/2}$	3046.697	4304.596	5788.186	7492.281	9419.742	11571.68	13949.44	16554.16
K	$^2P_{3/2}$	3046.837	4304.877	5788.681	7493.072	9420.909	11573.30	13951.57	16556.91
K	$^4P_{1/2}$	3055.555	4315.850	5801.737	7507.982	9437.387	11591.00	13970.09	16575.81
K	$^4P_{3/2}$	3055.724	4316.188	5802.348	7509.007	9439.014	11593.47	13973.71	16580.94
K	$^4P_{5/2}$	3055.942	4316.630	5803.151	7510.349	9441.110	11596.57	13978.10	16586.89

Table 2: Absolute values of the energy (E in $10^4 cm^{-1}$) for O-like systems. Designations: E=$1s^22s^22p^4$, F=$1s^22p^6$, C=$1s^22s2p^5$, I=$1s2s^22p^5$, K=$1s2s2p^6$

N	LSJ	$Z=12$	$Z=14$	$Z=16$	$Z=18$	$Z=20$	$Z=22$	$Z=24$	$Z=26$
E	$^3P_2$	4225.646	5976.973	8043.323	10419.92	13110.13	16115.68	19438.56	23080.73
E	$^3P_1$	4225.456	5976.554	8042.504	10418.45	13107.67	16111.75	19432.56	23071.88
E	$^3P_0$	4225.378	5976.394	8042.232	10418.06	13107.22	16111.42	19432.73	23073.16
E	$^1D_2$	4222.031	5972.297	8037.476	10412.72	13101.30	16104.81	19425.10	23063.94
E	$^1S_0$	4217.892	5967.002	8030.995	10404.98	13092.16	16094.00	19412.17	23048.21
C	$^3P_2$	4197.247	5940.518	7998.601	10366.63	13047.87	16043.88	19356.54	22987.61
C	$^3P_1$	4197.078	5940.145	7997.886	10365.38	13045.85	16040.81	19352.08	22981.41
C	$^3P_0$	4196.986	5939.944	7997.494	10364.68	13044.67	16038.92	19349.17	22977.03
C	$^1P_1$	4185.870	5926.373	7981.640	10346.75	13024.92	16017.64	19326.69	22953.72
F	$^1S_0$	4158.585	5891.295	7938.581	10295.47	12965.10	15948.94	19248.71	22866.02
I	$^3P_0$	3207.524	4561.043	6162.524	8007.970	10098.58	12436.31	15022.67	17859.08
I	$^3P_1$	3207.718	4561.432	6163.234	8007.970	10098.58	12436.31	15022.67	17859.08
I	$^3P_2$	3208.004	4562.005	6164.260	8009.653	10101.16	12440.02	15027.74	17865.68
I	$^1P_1$	3203.409	4555.788	6156.323	7999.842	10089.24	12425.65	15010.42	17844.70
K	$^1S_0$	3171.617	4515.824	6107.959	7942.803	10023.21	12350.30	14925.43	17749.79
K	$^3S_1$	3178.780	4525.024	6119.232	7956.190	10038.76	12368.06	14945.46	17772.16

Table 3: Absolute values of the energy (E in $10^4 cm^{-1}$) for F-like systems. Designations: E=$1s^22s^22p^5$, C=$1s^22s2p^6$, I=$1s2s^22p^6$

N	LSJ	$Z=12$	$Z=14$	$Z=16$	$Z=18$	$Z=20$	$Z=22$	$Z=24$	$Z=26$
E	$^2P_{3/2}$	4313.938	6142.588	8308.343	10806.40	13640.12	16811.20	20321.64	24173.43
E	$^2P_{1/2}$	4313.703	6142.062	8307.314	10804.58	13637.10	16806.49	20314.60	24163.28
C	$^2S_{1/2}$	4282.778	6102.162	8257.820	10745.74	13568.86	16728.78	20227.29	24065.98
I	$^2S_{1/2}$	3296.441	4734.311	6438.257	8408.919	10648.28	13156.65	15935.70	18978.92