Complete Atomic Data Base for Autoionizing Levels of B-like ions with $Z = 6 - 54$

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1 Introduction

In this paper, we calculate the autoionization decay of doubly excited $1s2s^22p^2, 1s2s2p^3, and 1s2p^4$ states via channels $1s^22s^2\,{}^1S$; $1s^22s2p\,{}^1P$, ${}^3P$; and $1s^22p^2\,{}^3P$, ${}^1D$, ${}^1S$ of B-like ions for a broad range of nuclear charge $Z = 6 - 54$. Recently, absolute energies of the autoionizing and non-autoionizing (ground and singly excited) levels and the total autoionization rates have been calculated for Li-, Be- and B-like ions with $Z = 6 - 54$ using the MZ method [1]. Not only the total autoionization rates, but also the amplitudes and rates of autoionization decay via channels, so-called partial rates, are very important in atomic kinetic calculations, for the modeling of dielectronic satellite spectra and, in particular, for polarization spectroscopy of astrophysical and laboratory high-temperature plasmas.

2 Calculational Methods

In the present paper we use two different calculational methods, namely MZ (the perturbation theory method) and AUTOLSJ (SUPERSTRUCTURE including configuration interaction). Earlier, we compared non-relativistic and relativistic energies calculated by these two methods for 4 to 10 electron systems of Ar and Fe ions [2].

2.1 MZ Code

The perturbation theory method is the basis of the MZ code developed by Vainshtein and Safronova [3, 4]. This method uses Z-expansions to calculate various atomic characteristics. The energy matrix is constructed in the LS-coupling scheme, including non-relativistic and relativistic parts. The non-relativistic part takes into account three or four terms of the Z-expansion. The relativistic part is constructed using Breit-Pauli operators. In the first step all these terms are calculated for diagonal and nondiagonal elements. In the second step, the energy matrix is diagonalized. The energies (eigen values) and the mixing coefficients (eigen vectors, C^J) are obtained. In the third step these mixing coefficients are used to obtain all the matrix elements in the intermediate coupling scheme. In the intermediate coupling scheme the partial autoionization rate A^{aut} in decay channel i can be expressed through amplitudes γ [1] (in a.u.):

$$A_i^{aut}(QLSJ, Q_i) = 2\sqrt{2}\pi \sum_{Q_1 Q_2 L_1 S_1} C^J(QLS, Q_1 L_1 S_1)\, \gamma(Q_1 L_1 S_1, Q_i L_1 S_1) \times \qquad (1)$$
$$\times \gamma(Q_i L_1 S_1, Q_2 L_1 S_1)\, C^J(Q_2 L_1 S_1, QLS)$$

Here $QLSJ$ are the quantum numbers characterizing the autoionizing level, Q_i is relevant to the channel i, $C^J(QLS, Q_1 L_1 S_1)$ are eigenvectors mentioned above, and 1 a.u.=$4.134 \times 10^{16}\ s^{-1}$. To calculate the total autoionization rates A_{tot}^{aut} we must sum up the partial rates A_i^{aut} over all decay channels.

2.2 AUTOLSJ Code

The AUTOLSJ package coordinates the calculation of energy levels, as well as radiative and autoionization rates. In the first step, the code determines non-relativistic wavefunctions by diagonalization of the non-relativistic hamiltonian on a set of chosen configurations. The single-electron wavefunctions are calculated in "scaled" Thomas-Fermi-Dirac-Amaldi potentials which are different for each angular momentum l. The scaling parameters are iterated to give the minimum energy of a term or of a group of terms. These potentials depend closely on the configurations. In our case two complexes $1s2s^22p^k$ + $1s2p^{k+2}$ and $1s2s2p^{k+1}$ are considered. To derive the non-relativistic and relativistic energies, the program diagonalizes the matrices relevant to the corresponding operators. In the second step (part of the AUTOLSJ package developed by Dubau et al 1981 [5]) we use the level mixing coefficients obtained by the energy matrix diagonalization to calculate the data.

3 Results

In Tables 1 and2 the results of our calculations of partial rates are presented for six decay channels, namely $1s^22s^2\ ^1S$; $1s^22s2p\ ^1P$, ^3P , and $1s^22p^2\ ^1S$, ^3P, ^1D, respectively. They are computed by the MZ (a) and AUTOLSJ (b) codes. Also, for comparison we use the Cowan program [6] and the data by Chen et al [7]. Thus, we compare the data (both partial and total autoionization rates) from four different codes. The comparison is, in general, good. Nevertheless, some disagreements appear due to levels with relatively weak autoionization rates ($< 10^{13} s^{-1}$). Moreover, we study the Z-dependences of partial rates for each complex of autoionizing levels with $J = 1/2, 3/2$ and $5/2$. In general, they show smooth trends. But the Z-dependences for levels with $J = 3/2$ of the configuration $1s2s2p^3$ (with a maximum value of eight levels in one complex) have a non-smooth form with maxima and minima.

References

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Table 1: Partial autoionization rates of B-like Fe decaying via the channels $1s^22s^2\ ^1S$, $1s^22s2p\ ^1P$ and $1s^22s2p\ ^3P$, calculated by MZ (a) and AUTOLSJ (b) codes. Designations: $I = 1s2s^22p^2$, $J = 1s2p^4$, $K = 2p^3[^4S]2s[^5S]1s$, $T = 2p^3[^4S]2s[^3S]1s$, $K = 2p^3[^2P]2s[^3P]1s$, $Q = 2p^3[^2P]2s[^1P]1s$, $K = 2p^3[^2D]2s[^3D]1s$, $Q = 2p^3[^2D]2s[^1D]1s$

		$1s^22s^2\ ^1S$		$1s^22s2p\ ^1P$		$1s^22s2p\ ^3P$	
Level	J	a	b	a	b	a	b
$1I$	1/2	0.691	1.112	2.63	2.43	2.93	2.33
$2I$	1/2	0.520	0.7190	0.715	0.609	14.6	12.3
$4I$	1/2	6.14	8.213	8.22	6.73	2.55	2.20
$5J$	1/2	0.0679	0.0025	0.110	0.103	0.189	0.0417
$6J$	1/2	0.0422	0.0041	0.0549	0.0513	0.187	0.160
$8J$	1/2	0.329	0.0026	0.432	0.3424	0.109	0.0929
$11K$	1/2	0	0	0.512	0.409	21.6	21.7
$13K$	1/2	0	0.0002	0.0422	0.0029	20.8	17.0
$14K$	1/2	0	0.0844	1.25	1.061	19.2	14.0
$17T$	1/2	0	0.0996	0.949	6.33	0.181	0.409
$18Q$	1/2	0	0.2667	18.0	9.05	2.07	3.09
$1I$	3/2	4.15	3.112	3.77	3.17	2.44	1.92
$2I$	3/2	0.0917	0.0648	0.0723	0.058	15.6	13.2
$3I$	3/2	14.1	11.31	8.12	6.86	2.09	1.80
$5J$	3/2	0.101	0.0038	0.0719	0.0569	0.0312	0.0253
$6J$	3/2	0.0098	0.00059	0.0079	0.0135	0.225	0.191
$7J$	3/2	0.187	0.0002	0.117	0.101	0.0463	0.0427
$10K$	3/2	0	0.0038	1.35	0.0429	6.36	5.05
$11K$	3/2	0	0	0.414	0.228	18.9	18.6
$12K$	3/2	0	0.0447	4.40	0.920	13.8	19.06
$13K$	3/2	0	0.0017	3.41	0.0778	14.1	15.8
$14K$	3/2	0	0.0019	10.6	11.3	10.5	7.74
$15Q$	3/2	0	0.0014	17.6	13.2	15.1	6.13
$16T$	3/2	0	0.0190	0.828	1.55	6.36	3.15
$18Q$	3/2	0	0.3050	17.6	12.5	1.43	3.42
$2I$	5/2	2.29	1.660	1.24	0.955	14.1	12.0
$3I$	5/2	16.1	12.82	8.71	7.30	3.70	3.19
$6J$	5/2	0.0082	0.00228	0.0045	0.0176	0.285	0.247
$7J$	5/2	0.286	0.0040	0.115	0.117	0.0316	0.0322
$9K$	5/2	0	0	0.005	0.005	0.708	0.549
$11K$	5/2	0	0	0.095	0.095	21.7	21.3
$12K$	5/2	0	0	0.433	0.125	21.7	21.2
$13K$	5/2	0	0	1.19	1.06	19.6	17.1
$15K$	5/2	0	0	20.5	21.7	1.66	1.03
$11K$	7/2	0	0	0	0	22.3	23.4

Table 2: Partial autoionization rates of B-like Fe decaying via the channels $1s^2 2p^2\ ^1S$, ^3P and ^1D, calculated by MZ (a) and AUTOLSJ (b) codes. Designations: $I = 1s2s^2 2p^2$, $J = 1s2p^4$, $K = 2p^3[^4S]2s[^5S]1s$, $T = 2p^3[^4S]2s[^3S]1s$, $K = 2p^3[^2P]2s[^3P]1s$, $Q = 2p^3[^2P]2s[^1P]1s$, $K = 2p^3[^2D]2s[^3D]1s$, $Q = 2p^3[^2D]2s[^1D]1s$

		$1s^2 2p^2\ ^1S$		$1s^2 2p^2\ ^3P$		$1s^2 2p^2\ ^1D$	
Level	J	a	b	a	b	a	b
$1I$	1/2	1.38	0.934	8.52	9.15	0.146	0.145
$2I$	1/2	1.01	0.588	8.76	12.1	0.093	0.080
$4I$	1/2	12.6	7.07	1.57	1.80	1.51	1.22
$5J$	1/2	0.749	0.735	29.7	22.3	4.07	3.86
$6J$	1/2	0.338	0.318	32.1	24.5	2.00	1.81
$8J$	1/2	4.54	3.71	7.24	6.24	23.3	18.6
$11K$	1/2	0.071	0.051	0.228	2.19	0.088	0.068
$13K$	1/2	0.051	0.003	2.63	2.23	0.006	0.004
$14K$	1/2	0.218	0.166	9.09	7.76	0.272	0.214
$17T$	1/2	0.214	1.69	10.5	5.45	0.268	2.23
$18Q$	1/2	7.60	4.60	4.11	6.66	9.50	6.07
$1I$	3/2	0.031	0.072	7.19	8.33	2.17	2.37
$2I$	3/2	3.0-4	0.002	9.35	10.3	0.048	0.044
$3I$	3/2	0.068	0.336	2.19	2.24	7.34	8.19
$5J$	3/2	2.60	1.96	20.0	16.6	19.8	13.6
$6J$	3/2	0.107	0.243	34.0	25.2	0.826	1.59
$7J$	3/2	3.43	3.14	15.2	10.9	26.3	21.3
$10K$	3/2	0.234	0.067	4.56	3.10	0.829	0.118
$11K$	3/2	0.003	0.01	0.866	2.06	0.115	0.029
$12K$	3/2	0.455	0.778	5.18	9.63	6.54	3.27
$13K$	3/2	0.257	0.031	4.50	4.38	1.42	0.044
$14K$	3/2	1.86	0.025	7.33	4.19	8.09	6.50
$15Q$	3/2	0.227	0.029	3.28	4.10	1.90	5.80
$16T$	3/2	0.311	0.325	18.3	18.8	1.93	0.432
$18Q$	3/2	4.76	5.24	2.51	6.63	7.55	7.85
$2I$	5/2	0.009	0.059	8.19	9.25	1.19	1.16
$3I$	5/2	0.089	0.356	1.15	1.28	8.36	9.42
$6J$	5/2	0.046	0.325	34.4	24.6	0.363	2.09
$7J$	5/2	6.10	5.01	0.265	1.58	46.5	34.4
$9K$	5/2	0	0	0.091	0.072	0.002	0.001
$11K$	5/2	0	0	0.468	2.19	0.025	0.019
$12K$	5/2	0	0	0.225	9.05	1.24	1.86
$13K$	5/2	0	0	1.89	2.22	0.212	0.137
$15Q$	5/2	0	0	0.098	0.583	16.8	13.4
$11K$	7/2	0	0	0	2.21	0	0