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CONTENTS

DIELECTRONIC RECOMBINATION RATE COEFFICIENTS FOR IONS OF THE Be AND B ISONUCLEAR SEQUENCES

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ABSTRACT. Dielectronic recombination rate coefficients for all ions of the Be and B isonuclear sequences are calculated in the zero density limit using a multiconfiguration, intermediate coupling approximation for atomic structures.

The appearance of low-Z metals in current tokamak fusion experiments has prompted the IAEA to extend its atomic database to cover these materials. In this paper we calculate dielectronic recombination (DR) rate coefficients for all atomic ions of the beryllium and boron isonuclear sequences. The zero density rates generated here need to be incorporated into the solution of the collisional-dielectronic population rate equations [1] from which level populations, ionization balance and power loss can be determined for a finite density plasma.

The energy averaged dielectronic recombination cross-section for a given initial state i through an intermediate state j is given by

$$\bar{\sigma}_d(i \to j) = \frac{(2\pi a_0 I)^2}{E_c \Delta E_c} \frac{\omega(j)}{2\omega(i)} \times \frac{\tau_0 \sum_k A_r(j \to k) \sum_\ell A_a(j \to i, E_c \ell)}{\sum_h \left[A_r(j \to h) + \sum_\ell A_a(j \to h, E_c \ell) \right]} \qquad (1)$$

where E_c is the energy of the continuum, which is fixed by the position of the resonances, I is the ionization potential of hydrogen and ΔE_c is the bin width. $\omega(j)$ is the statistical weight of the (N + 1) electron doubly excited state, $\omega(i)$ is the statistical weight of the N-electron target ion, and $(2\pi a_0)^2 \tau_0 = 2.6741 \times 10^{-32}$ cm^2·s. The dielectronic recombination rate coefficient can be written in terms of the energy averaged cross-section as

$$\alpha_d(i) = \left[\frac{4\pi a_0^2 I}{k_B T} \right]^{3/2} \frac{1}{(2\pi a_0 I)^2 \tau_0} \times \sum_j E_c \Delta E_c \bar{\sigma}_d(i \to j) \exp(-E_c/k_B T) \qquad (2)$$

where $(4\pi a_0^2)^{3/2} = 6.6011 \times 10^{-24}$ cm^3. Many-body perturbation theory is used to evaluate both the radiative (A_r) and the autoionization (A_a) rates for the many intermediate levels j in the energy range of interest. The atomic structure computer code SUPERSTRUCTURE [2], based on Thomas–Fermi–Dirac–Amaldi (TFDA) wave functions, was extensively modified to calculate multiconfiguration, intermediate coupling autoionization rates. The resulting computer code AUTOSTRUCTURE [3, 4] calculates multiconfiguration, intermediate coupled DR cross-sections, Eq. (1), and rate coefficients, Eq. (2), for low n explicitly and for high n by extrapolating radial wave functions using quantum defect theory.

For dielectronic recombination in B^+, we consider the following reaction pathways ($1s^2$ core):

$$(2s^2 + 2p^2)\,{}^1S_0 + k\ell_c \to 2s2p({}^3P_{2,1,0}, {}^1P_1)n\ell \qquad (3)$$

$$\begin{aligned} 2s2p({}^3P_{2,1,0}, {}^1P_1)n\ell &\to (2s^2 + 2p^2)\,{}^1S_0 n\ell + \hbar\omega \\ &\searrow (2s^2 + 2p^2)\,{}^1S_0 + k\ell_c \\ &\searrow 2s2p({}^3P_{2,1,0}, {}^1P_1) + k'\ell'_c \end{aligned} \qquad (4)$$

where we sum the above processes up to n = 1000 and $\ell = 12$. The DR rate coefficients for B^+ from 10^4 K to 10^8 K are given in Table II.

For dielectronic recombination in Be^+ and B^{2+}, we consider the following reaction pathways ($1s^2$ core):

$$2s\,{}^2S_{1/2} + k\ell_c \to 2p({}^2P_{3/2,1/2})n\ell \qquad (5)$$

$$\begin{aligned} 2p({}^2P_{3/2,1/2})n\ell &\to 2s\,{}^2S_{1/2}n\ell + \hbar\omega \\ &\searrow 2s\,{}^2S_{1/2} + k\ell_c \\ &\searrow 2p({}^2P_{3/2,1/2}) + k'\ell'_c \end{aligned} \qquad (6)$$

where we sum the above processes up to n = 1000 and $\ell = 12$. The DR rate coefficients for Be^+ and B^{2+}

TABLE I. Be DIELECTRONIC RECOMBINATION RATE COEFFICIENTS

$\log_{10}$ [T(K)]	Be^{+} α (10^{-11} cm^3/s)	Be^{2+} α (10^{-11} cm^3/s)	Be^{3+} α (10^{-11} cm^3/s)
4.0	0.62872		
4.1	1.15464		
4.2	1.74627		
4.3	2.26130		
4.4	2.58738		
4.5	2.68276		
4.6	2.57202		
4.7	2.31695		
4.8	1.98634		
4.9	1.63721		
5.0	1.30790		
5.1	1.01920		
5.2	0.77871		
5.3	0.58570	0.00184	0.00125
5.4	0.43508	0.00531	0.00574
5.5	0.32002	0.01151	0.01811
5.6	0.23354	0.01987	0.04222
5.7	0.16937	0.02858	0.07727
5.8	0.12222	0.03556	0.11649
5.9	0.08785	0.03942	0.15046
6.0	0.06295	0.03986	0.17182
6.1	0.04500	0.03746	0.17789
6.2	0.03210	0.03321	0.17035
6.3	0.02286	0.02812	0.15332
6.4	0.01626	0.02295	0.13136
6.5	0.01156	0.01819	0.10821
6.6	0.00821	0.01408	0.08641
6.7	0.00582	0.01071	0.06732
6.8	0.00413	0.00802	0.05142
6.9	0.00293	0.00594	0.03867
7.0	0.00208	0.00436	0.02872
7.1	0.00147	0.00317	0.02112
7.2	0.00104	0.00230	0.01541
7.3		0.00166	0.01118
7.4		0.00119	0.00807
7.5			0.00580
7.6			0.00415
7.7			0.00297
7.8			0.00212
7.9			0.00151
8.0			0.00107

from 10^4 K to 10^8 K are given in Tables I and II, respectively.

For dielectronic recombination in Be^{2+} and B^{3+}, we consider the following reaction pathways:

$$1s^2\,{}^1S_0 + k\ell_c \rightarrow 1s2\bar{\ell}({}^3S_1, {}^1S_0, {}^3P_{2,1,0}, {}^1P_1)n\ell \tag{7}$$

$$\begin{aligned} 1s2\bar{\ell}({}^3S_1, {}^1S_0, {}^3P_{2,1,0}, {}^1P_1)n\ell \rightarrow\ & 1s^2\,{}^1S_0 2\bar{\ell} + \hbar\omega \\ \searrow\ & 1s^2\,{}^1S_0 n\ell + \hbar\omega \\ \searrow\ & 1s^2\,{}^1S_0 + k\ell_c \\ \searrow\ & 1s2\bar{\ell}({}^3S_1, {}^1S_0, {}^3P_{2,1,0}, {}^1P_1) + k'\ell_c' \end{aligned} \tag{8}$$

where we sum the above processes up to n = 100 and ℓ = 5. The DR rate coefficients for Be^{2+} and B^{3+} from 10^4 K to 10^8 K are given in Tables I and II, respectively. For B^{3+}, the peak DR rate coefficient (at 1.6×10^6 K) calculated by Chen [5] is about 8% lower than the value given in Table II.

For dielectronic recombination in Be^{3+} and B^{4+}, we consider the following reaction pathways:

$$1s\,{}^2S_{1/2} + k\ell_c \rightarrow 2\bar{\ell}({}^2S_{1/2}, {}^2P_{3/2,1/2})n\ell \tag{9}$$

$$\begin{aligned} 2\bar{\ell}({}^2S_{1/2}, {}^2P_{3/2,1/2})n\ell \rightarrow\ & 1s\,{}^2S_{1/2} 2\bar{\ell} + \hbar\omega \\ \searrow\ & 1s\,{}^2S_{1/2} n\ell + \hbar\omega \\ \searrow\ & 1s\,{}^2S_{1/2} + k\ell_c \\ \searrow\ & 2\bar{\ell}\,{}^2S_{1/2}, {}^2P_{3/2,1/2} + k'\ell_c' \end{aligned} \tag{10}$$

where we sum the above processes up to n = 100 and ℓ = 5. The DR rate coefficients for Be^{3+} and B^{4+} from 10^4 K to 10^8 K are given in Tables I and II, respectively.

In conclusion, we have generated zero density DR rate coefficients for all atomic ions of the Be and B isonuclear sequences. The rates generated here are the first step in the solution of the collisional-dielectronic population rate equations for a finite density plasma. The overall accuracy of the DR rates is judged to be about 20%, because of approximations in the atomic structure and the neglect of contributions from higher excitations.

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TABLE II. B DIELECTRONIC RECOMBINATION RATE COEFFICIENTS

$\log_{10}$ [T(K)]	B^+ α (10^{-11} cm^3/s)	B^{2+} α (10^{-11} cm^3/s)	B^{3+} α (10^{-11} cm^3/s)	B^{4+} α (10^{-11} cm^3/s)
4.0	0.00171	0.22968		
4.1	0.01272	0.56034		
4.2	0.05879	1.16283		
4.3	0.18535	1.98648		
4.4	0.43052	2.85670		
4.5	0.78384	3.56351		
4.6	1.17568	3.96259		
4.7	1.51149	4.01867		
4.8	1.71906	3.78663		
4.9	1.77367	3.36497		
5.0	1.69369	2.85402		
5.1	1.52082	2.33252		
5.2	1.30046	1.85090		
5.3	1.06968	1.43469		
5.4	0.85312	1.09155		
5.5	0.66394	0.81827	0.00353	0.00152
5.6	0.50674	0.60624	0.01061	0.00652
5.7	0.38083	0.44497	0.02387	0.01959
5.8	0.28271	0.32418	0.04247	0.04411
5.9	0.20783	0.23479	0.06266	0.07863
6.0	0.15160	0.16926	0.07959	0.11620
6.1	0.10991	0.12156	0.08972	0.14781
6.2	0.07929	0.08705	0.09195	0.16680
6.3	0.05699	0.06219	0.08735	0.17110
6.4	0.04083	0.04434	0.07813	0.16267
6.5	0.02918	0.03157	0.06661	0.14558
6.6	0.02081	0.02245	0.05466	0.12416
6.7	0.01482	0.01595	0.04351	0.10192
6.8	0.01054	0.01133	0.03381	0.08116
6.9	0.00749	0.00804	0.02578	0.06309
7.0	0.00532	0.00570	0.01936	0.04811
7.1	0.00378	0.00404	0.01436	0.03613
7.2	0.00268	0.00286	0.01055	0.02680
7.3	0.00190	0.00203	0.00769	0.01969
7.4	0.00135	0.00144	0.00558	0.01436
7.5		0.00102	0.00402	0.01041
7.6			0.00289	0.00751
7.7			0.00207	0.00539
7.8			0.00148	0.00386
7.9			0.00105	0.00276
8.0				0.00197

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