Dielectronic recombination into Mg-like ions

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Abstract. Dielectronic recombination (DR) rate coefficients for Na-like ions forming Mg-like ions of Fe, Zn, Kr, and Mo are calculated. Energy levels, radiative transition probabilities, and autoionization rates for 1s2s2p63\textit{l}n\textit{l}, 1s2s2p44\textit{l}n\textit{l}, and 1s2s2p33\textit{l}n\textit{l} states are calculated by using the Hartree-Fock-relativistic method (Cowan code). Total and state-selective DR rate coefficients are derived as a function of electron temperature. Configuration mixing plays an important role for DR rates of 1s2s2p63\textit{l}n\textit{l} states. Energy level structure near the first 3s threshold is important for DR rate coefficients behaviour at low temperature.

1. Introduction

Dielectronic recombination (DR) is important process governing ionization state of ions in various plasmas. Many theoretical and experimental studies on DR have been done for K-shell and L-shell ions, but not so many for M-shell ions. Recently Netzer [1] and Kraemer et al. [2] suggested importance of M-shell Fe ions and the data needs for astrophysical plasmas such as photoionized plasma of active galactic nuclei. The solar observational satellite HINODE was launched in 2006 and has EUV Imaging Spectrometer (EIS) to observe the sun with EUV spectral lines of Fe M-shell ions [3]. Plasma diagnostics by using spectral lines of Fe ions will provide information on the active region and the transition region of the sun to study the coronal heating problem. Reliable data of total and state-selective DR rate coefficients are needed for determining ionization state of ions and level populations to estimate spectral line intensities for plasma diagnostics.

Here we focus on DR process forming Mg-like ions. The DR rate coefficients are calculated including 1s2s2p63\textit{l}n\textit{l}, 1s2s2p44\textit{l}n\textit{l}, and 1s2s2p33\textit{l}n\textit{l} states in Mg-like iron (Fe14\textsuperscript{+}), Mg-like Zn (Zn18\textsuperscript{+}), Mg-like Kr (Kr24\textsuperscript{+}) and Mg-like Mo (Mo30\textsuperscript{+}) ions. The energy levels, transition probabilities and autoionization rates required for calculating the DR rate coefficients are determined. The present paper continues our efforts on calculation of the low-temperature DR rate coefficients for CI [4], CII [5,6], CIII [7], OIII [8], OIV [9], OV [10], Ne VII [11], and Fe XV [12]. In paper [12] we did not include 1s2s2p33\textit{l}n\textit{l} states which contribute to the DR rate coefficient at high temperature. Hereafter we omit the core 1s2s2 from the configuration notation.

2. Atomic data

Atomic parameters for intermediate and final states of DR processes are needed to determine the DR rate coefficients. We calculated energy levels, radiative transition probabilities, and autoionization rates for 2p63\textit{l}n\textit{l} (n = 3-\textit{n}_\text{I}, l < 8), 2p44\textit{l}n\textit{l} (n = 4-7, l < n), and 2p33\textit{l}n\textit{l} (n = 3-4, l < n) states in Fe14\textsuperscript{+}, Zn18\textsuperscript{+}, Kr24\textsuperscript{+} and Mo30\textsuperscript{+} ions by using the Hartree-Fock-Relativistic method (Cowan code [13,14]). The upper limit of \textit{n} for calculating 2p63\textit{l}n\textit{l} states, \textit{n}_\text{I}, is set as 12 for Fe14\textsuperscript{+} and Zn18\textsuperscript{+}, 13 for Kr24\textsuperscript{+} and 14
for Mo$^{30+}$. Due to computational issues, calculation of the DR parameters involving 2p$^64l'nl$ states was performed with account of 2p$^63l'nl$ states with $n \leq 8$ only, and calculation of the DR parameters involving 2p$^53l''3l'n'l$ states, with account of 2p$^63l'nl$ states with $n \leq 5$ only. We use one scaling factor (0.85) for all electrostatic integrals in the Cowan code. Radiative transition probabilities with $A_r < 10^5$ s$^{-1}$ were omitted from consideration for simplicity.

Autoionizing states are the 2p$^63p$nl states with $n \geq 10$ (Fe$^{14+}$), 11 (Zn$^{18+}$), or 12 (Kr$^{24+}$ and Mo$^{30+}$) and the 2p$^33dn'l$nl states with $n \geq 7$ (Fe$^{14+}$ and Zn$^{18+}$), 8 (Kr$^{24+}$), or 9 (Mo$^{30+}$). Some of 2p$^64l'nl$ states listed in Table 1 are located below the first 3s threshold and are not autoionizing. All 2p$^64l'nl$ states with $n = 4-7$ are below the third 3d threshold for these ions.

| Ion       | I$_{3s}$ (cm$^{-1}$) | states                                                                 |
|-----------|----------------------|----------------------------------------------------------------------|
| Fe$^{14+}$| 3,686,000            | 2p$^6$4s$^2$1S$_0$, 2p$^6$4s$^4$p$^3$P$_{0,1,2}$, 2p$^6$4p$^2$3P$_{0,1,2}$ |
| Zn$^{18+}$| 5,670,000            | 2p$^6$4s$^2$1S$_0$, 2p$^6$4s$^4$p$^3$P$_{0,1,2}$, 2p$^6$4p$^2$3P$_{0,1,2}$ |
| Kr$^{24+}$| 9,315,400            | 2p$^6$4s$^2$1S$_0$, 2p$^6$4s$^4$p$^3$P$_{0,1,2}$, 2p$^6$4p$^2$3P$_{0,1,2}$ |
| Mo$^{30+}$| 13,920,000           | 2p$^6$4s$^2$1S$_0$, 2p$^6$4s$^4$p$^3$P$_{0,1,2}$, 2p$^6$4p$^2$3P$_{0,1,2}$ |

3. Dielectronic recombination rate coefficients

The DR rate coefficients are obtained by the following equations:

$$\alpha_r(i_0, j) = 3.3 \times 10^{-24} \left( \frac{I_m}{kT_e} \right)^{3/2} \frac{1}{g_0} \sum_i Q_j(j,i) \exp \left( \frac{-E_i(j)}{kT_e} \right),$$

$$Q_j(j,i) = \sum_{i_0} g(i) A_u(i,i_0) A_r(j,i) \sum_k A_r(k,i),$$

where $i_0$ indicates initial state, $j$ final state, $i$ intermediate autoionizing state. $I_m$ is hydrogen ionization potential energy, $T_e$ electron temperature, $E_i(j)$ energy from ionization threshold, $g_0$ and $g(i)$ statistical weights of initial state and $i$ state, $A_u$ autoionization rate, and $A_r$ radiative transition probability.

The contributions from the high $n$ autoionizing states to the DR rate coefficients are estimated by using empirical scaling laws [4] for atomic parameters. The one-electron dipole transitions, eg., 3s-np, 3p-ns, 3p-nd, 3d-np, and 3d-nf, are taken into account. Details are described in [12]. In addition 2p-nl transitions are also taken into account in this paper. The $1/n^3$ scaling law for $A_u$ and $A_r$ is used. The high $n$ state contributions up to $n=1000$ are calculated.

The state-selective and total DR rate coefficients are derived as a function of electron temperature. Figures 1(a)-(d) show the total DR rate coefficients of Mg-like Fe, Zn, Kr and Mo ions. Contributions of 2p$^63ln'l'$, 2p$^64ln'l'$, and 2p$^53ln'l'n''l''$ states to the DR rate coefficients are also shown. Figure 2 shows examples of state-selective DR rate coefficients in Mg-like Fe. Contributions of 2p$^53ln'l'n''l''$ states are seen at $T_e > 100$eV.

Configuration mixing for 2p$^6$ [3snp + 3pnp + 3dnd], 2p$^6$ [3snp + 3pns + 3pnd + 3dmp] and 2p$^6$ [3snd + 3pnp + 3pnt + 3dns + 3dng] states plays an important role for the DR rate coefficients of 3snl levels with low $n$ at low temperature. For example, 2p$^6$ [3s$^2$ + 3p$^2$ + 3d$^2$] (all), 2p$^6$ [3s6p + 3p5d + 3p6s + 3d5p] (Mg-like Fe), 2p$^6$ [3s7s + 3p6p + 3d5d] (Mg-like Zn), 2p$^6$ [3s5d + 3p5p + 3p5f + 4d5s] (Mg-like Mo) show configuration mixing.

The total DR rate coefficients agree well with previously published data by Gu [15], Altun et al. [16], and Fournier et al. [17] (Mg-like Mo) except for low temperature region. The behavior of the DR rate coefficients at low temperature strongly depends on the energy level structure. DR processes through autoionizing levels just above the first 3s threshold contribute to the DR rate coefficients at
high temperature. For Mg-like Fe, $2p^63p10l$ and $2p^64s4p$ states are located near the 3s threshold and DR processes through these states contribute to the DR rate at low temperature. The $2p^63d7l$ states for Mg-like Zn, the $2p^63d8l$ and $2p^63p12l$ states for Mg-like Kr and the $2p^64p4l$ states for Mg-like Mo locate close to the 3s threshold, respectively and contribute to the DR rate coefficients at low temperature. These different level structures cause different behavior of the DR rate coefficients.

![Figure 1](image1.png)

**Figure 1.** Dielectronic recombination rate coefficient in Mg-like Fe (a), Zn (b), Kr (c), and Mo (d) as a function of electron temperature. Contributions of transitions through $2p^63nl$, $2p^64nl$ and $2p^63lnl’$ states are shown. Results by Altun et al. [16], Gu [15] and Fournier et al. [17] are also shown for comparison.

![Figure 2](image2.png)

**Figure 2.** Dielectronic recombination rate coefficient for the $3/3l’$ states as a function of electron temperature in Mg-like Fe.
Contributions of high $n$ states become important at $T_e > 10-30 \text{eV}$ and contributions of $2p$-$nl$ transitions through $2p^53ln'ln''l''$ become important at $T_e > 200-600 \text{eV}$.

4. Conclusion
In this paper we calculate a large set of atomic data related to DR processes of Na-like ions into Mg-like ions of Fe, Zn, Kr and Mo. Energy levels, radiative transition probabilities and autoionization rates are calculated for Mg-like Fe, Zn, Kr, and Mo ions by using the Hatree-Fock-relativistic method (Cowan code). The calculated atomic data are used to obtain the DR rate coefficients. We take into account doubly excited states $2p^53ln'l'$ and $2p^44ln'l'$ and inner-shell excited states $2p^53ln'l'n''l''$ as intermediate states with $n$ up to 1000 to calculate the DR rate coefficients.

Configuration mixing plays an important role for the DR rate coefficients of $3snl$ states with low $n$. The autoionizing states which located close to the first $3s$ threshold contribute to the DR rate coefficient at low temperature, which strongly depends on the energy level structure of each ion. The DR rate coefficients are in good agreement with previously published data at medium and high temperature.

The state selective rate coefficients can be used in collisional-radiative modelling for population kinetics and plasma diagnostics in recombining plasmas, which is important to examine behaviour and properties of non-equilibrium plasma such as the transition region of the sun.

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