NASA LAW, October 25-28, 2010, Gatlinburg

Dielectronic Recombination Calculations for Fe^{15+}

D.-H. Kwon[1] & D. W. Savin

Columbia Astrophysics Laboratory, Columbia University, New York, NY 10027, USA

dk2545@columbia.edu

ABSTRACT

Dielectronic recombination (DR) of Na-like Fe^{15+} forming Mg-like Fe^{14+} via excitation of a $2l$ core electron has been investigated. We find that configuration interaction (CI) between DR resonances with different captured electron principal quantum numbers n can lead to a significant reduction in resonance strengths for $n \geq 5$. Including this form of CI accounts for most of the discrepancy between previous theoretical and experimental results. Here we briefly present our results and discuss their implications for the modeling of cosmic plasmas.

1. Introduction

The physical properties of cosmic sources can be determined using spectral observations coupled with theoretical models. Spectral observations depend on ion and elemental abundances. In order to determine the fractional ionic abundances of the plasma one needs to know the rate coefficients for all relevant ionization and recombination processes. Dielectronic recombination (DR) is the dominant electron-ion recombination process for most ions in cosmic plasmas.

DR is a two-step recombination process which begins when a free electron collides with an ion of charge $q+$ and in initial state i. The incident electron collisionally excites a core electron of the ion with principal quantum number n and is simultaneously captured forming a system of state j. The energy of the intermediate system lies in the continuum and it may autoionize. DR occurs when the state j radiatively decays to a state f emitting a photon.

[1]Laboratory for Quantum Optics, Korea Atomic Energy Research Institute, Daejeon 305-600, Republic of Korea.

Here we address a particularly nagging discrepancy between theory and experiment for the relatively simple Na-like Fe^{15+} forming Mg-like Fe^{14+}. Good agreement between experiment and theory has been found for Fe^{15+} DR via $\Delta n_c = 0$ and 1 core excitations of a $3s$ electron (Linkemann et al. 1995; Gorczyca & Badnell 1996; Gu 2004; Altun et al. 2006). For $\Delta n_c = 1$ core excitations of $2l$ electron, previous theoretical work has shown the importance of configuration interaction (CI) within a $2s^2 2p^5 3l 3l' nl''$ complex (Gorczyca & Badnell 1996). Including this CI reduced the predicted overall resonance strength. However, all of these theoretical results consider CI only within the same n levels. Such results are still significantly larger than experiment for collision energies over 620 eV.

We have investigated the importance of CI between different n complexes of the captured electron for Fe^{15+} DR via $\Delta n_c = 1$ core excitations of $2l$ electron. We use the Flexible Atomic Code (FAC) which is based on a fully relativistic Dirac Hamiltonian equation and utilizes a distorted wave approximation. Here we present some of our results.

2. Theoretical method

We calculated DR using the independent process, isolated resonance (IPIR) approximation. This method treats radiative recombination and DR separately and neglects quantum mechanical interferences between the two and between DR resonances. The energy integrated cross section (i.e., resonance strength) of state j is given by Kilgus et al. (1992) in atomic units as

$$\hat{\sigma}_j = \frac{\pi^2}{E_j} \frac{g_j}{2g_i} \frac{A^a_{ji} \sum_f A^r_{jf}}{\sum_k A^a_{jk} + \sum_f A^r_{jf}}. \tag{1}$$

Here E_j is the resonance energy of the intermediate system, g_i and g_j are statistical weights, A^a_{ji} is the autoionization rate from j to an initial recombining state i, A^a_{jk} is the autoionization rate from j to any state k of A^{q+}, and A^r_{jf} is the radiative decay rate from j to f.

We considered the multiply-excited $2l^7 3l' 3l'' nl'''$ resonance states, thereby including $2s \to 3l$ promotion; the $2l^8 3l'$, $2l^8 nl'''$, and $2l^7 3l' 3l''$ autoionization decay channels; and the $2l^8 3l' 3l''$ and $2l^8 3l' nl'''$ radiative decay channels. The maximum angular momentum considered was 5. The $n > 6$ $2l^8 3l' nl'''$ levels lie in the continuum and radiative Decays to Autoionizing levels followed by radiative Cascades (DAC) are possible. The branching ratio for the DAC process is given by

$$B_j = \frac{\sum_t A^r_{jt} + \sum_{t'} A^r_{jt'} B_{t'}}{\sum_k A^a_{jk} + \sum_f A^r_{jf}}, \tag{2}$$

where the final states t and t' are below and above the ionization threshold, respectively. $B_{t'}$

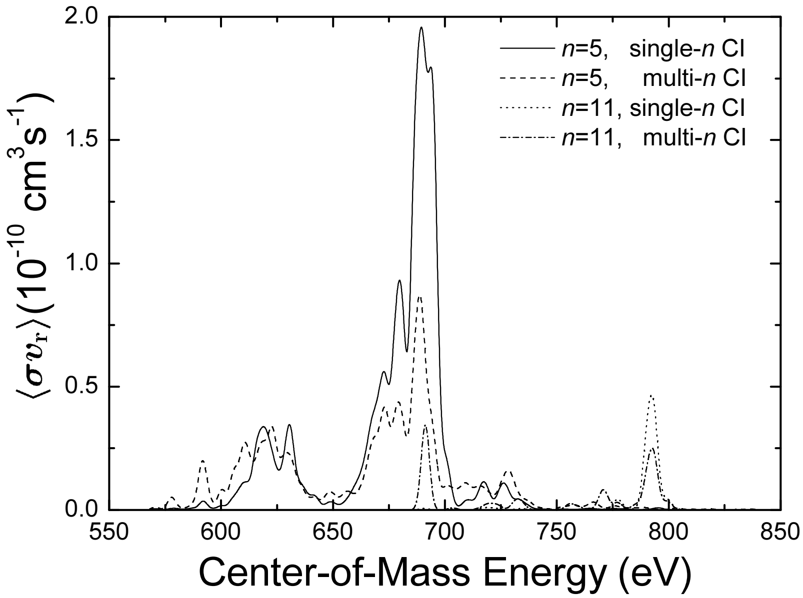

Fig. 1.— DR resonance structure of the $n = 5$ and $n = 11$ resonances for single-n and multi-n CI.

is the branching ratio for radiative stabilization of t' and can be determined by evaluating B_j iteratively.

We performed a large scale CI calculation including all $2l^7 3l' 3l'' nl'''$ complexes from $n = 3$ to 14. This allowed us to consider CI between resonances with different captured electron principal quantum numbers. Radial wave functions were optimized on the $2l^8 3l' 3l''$ configuration. We calculated autoionization and radiative decay rates from the wave functions obtained using this CI mixing.

3. Results

Figure 1 shows a DR resonance spectrum for $n = 5$ and $n = 11$. We plot here the DR cross section σ times the relative collision velocity $v_{\rm r}$ convolved with the experimental energy distribution of Linkemann et al. (1995) which was $k_{\rm B}T_{\parallel} = 2.4$ meV along the beams and $k_{\rm B}T_{\perp} = 0.1$ eV perpendicular to the beams. The $n = 5$ resonance spectrum peak is clearly reduced in strength when multi-n CI is considered. This behavior can be explained by configuration mixing of a strong resonance level in single-n CI with weak resonance levels of different n complexes. On the other hand, the weak $n = 11$ resonance level is largely enhanced by CI mixing with the strong $n = 5$ resonance levels. This can be seen around

~ 680 eV in Figure 1.

Multi-n CI can significantly reduce the theoretical DR resonances strength compared to single-n CI calculations. This brings theory into very good agreement with the experimental results of Linkemann et al. (1995) as is discussed in more detail in Kwon & Savin (in preparation). From our multi-n CI calculations we have derived a Maxwellian rate coefficient $\alpha_{\rm DR}$ needed for plasma modeling. Multi-n CI for $\Delta n_{\rm c} = 1$ core excitation of a $2l$ electron reduces the total Maxwellian rate coefficient by a maximum of about 15% at temperatures where Fe^{15+} forms in collisionally ionized gas.

4. Summary

We have demonstrated the importance of CI between resonances with different captured electron principal quantum numbers n for DR of Na-like Fe^{15+} forming Mg-like Fe^{14+} via $\Delta n_{\rm c} = 1$ core excitation of a $2l$ electron. Multi-n CI significantly reduces the theoretical resonance strengths for capture into $n \geq 5$ levels. This brings theory into very good agreement with experiment and removes a previously existing discrepancy between the two. CI between different n levels reduces the Maxwellian DR rate coefficient by a maximum of about 15% at temperatures where Fe^{15+} forms in collisional ionization equilibrium.

This work was supported in part by the NASA Astronomy and Physics Research and Analysis (APRA) Program.

REFERENCES

Linkemann, J., et al. 1995, Nucl. Instrum. Methods B, 98, 154.

Gorczyca, T., W., & Badnell, N. R. 1996, Phys. Rev. A, 54, 4113.

Gu, M., F. 2004, Astrophys. J. Suppl. Ser, 153, 389.

Altun, Z., et al. 2006, Astron. Astrophys., 447, 1165.

Kilgus, G., et al. 1992, Phys. Rev. A, 46, 5730.

Kwon, D.-H., & Savin, D. W., in preparation.

This preprint was prepared with the AAS LaTeX macros v5.2.