Unified Electron-Ion Recombination Cross Sections and Rates

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1 Introduction

Calculations of unified electron-ion recombination cross sections are described within the framework of the close coupling (CC) approximation using the R-matrix method. It is emphasized that the unified treatment subsumes and computationally unifies "radiative" recombination (RR) and "dielectronic" recombination (DR) processes. Calculations are carried out in non-relativistic and relativistic approximations for C V, C VI, O VIII and are compared with available accurate experimental measurements on ion storage rings and electron beam traps with very good agreement. Radiation damping of autoionizing resonances is included for these ions and found to be significant for H-like and He-like ions, although unlikely to be of importance in other ionic species. A comprehensive and self-consistent set of new atomic data of photoionization and recombination rate coefficients for oxygen ions is also obtained. These are for direct applications to astrophysical models. Sample results are presented. Complete datasets will be available electronically.

2 Theoretical Summary

Extending the CC approximation and the R-matrix method [1] to electron-ion recombination, and using the DR theory by Bell and Seaton (BS) [2], Nahar and Pradhan [3] have developed a computationally unified approach to obtain total e+ion recombination cross sections, σ_{RC}, and rate coefficients, $\alpha_R(T)$. The approach entails: (a) computation of photo-recombination cross sections from photoionization cross sections, σ_{PI}, for all bound states with $\nu \leq \nu_0 \approx 10$ (ν is the effective quantum number) via the Milne detailed-balance relation and (b) DR cross sections from radiatively damped high-n resonances, $\nu_0 < \nu \leq \infty$, using analytic expressions for both the detailed and the resonance averaged cross sections derived from the BS theory. The computations are highly involved and, for example, include in (a) σ_{PI} of several hundred bound states of the (e+ion) system with low-n autoionizing resonances (up to $\nu \approx \nu_0$) delineated at several thousand photon energies. This method yields *total* σ_{RC} in an *ab initio* and unified manner, including the background RR and the resonant DR. Physically, there is no separation between the two processes, therefore the present total (unified) cross sections can be compared directly with *absolute* experimental measurements in the entire energy range. The $\alpha_R(T)$ are obtained through maxwellian averaging over the recombination cross sections.

Experimental measurements of σ_{RC} for carbon and oxygen ions, C V, C VI, O VIII, using the Test Storage Ring (TSR) at Heidelberg, exhibit detailed resonance structures observed at very high resolution in beam energy [5]. The experiments measure absolute cross sections and therefore provide ideal tests for theoretical methods, as well as the physical effects included in the calculations. The present work aims to demonstrate the accuracy of the unified method for electron-ion recombination, on par with the CC treatment of photoionization and electron impact excitation, by comparing σ_{RC} with the measured values.

One additional consideration in the present work is the inclusion of radiation damping of low-*n* resonances of C IV, C V, and O VIII since damping of resonances is known to be important for highly charged H-like and He-like ions. The reason is that for the dipole allowed transitions, $2p \rightarrow 1s$ and $1s2p\ ^1P^0 \rightarrow 1s^2\ ^1S$ the radiative decay rates, Γ^r, of the order of 10^{13} - 10^{14} s^{-1}, approach typical autoionization rates, Γ^a, of 10^{14} s^{-1}. However, damping is negligible for all other ionization stages where for the outer core transitions such as $n = 3 \rightarrow 2$, or $n = 4 \rightarrow 3$, Γ^r is generally orders of magnitude smaller than Γ^a. Recently, employing the Breit-Pauli (BP) R-matrix method (BPRM) [4], the calculations of recombination have been extended to highly charged ions including the BP relativistic effects and radiation damping [6]. We implement this new extension to C V, C VI, and O VIII.

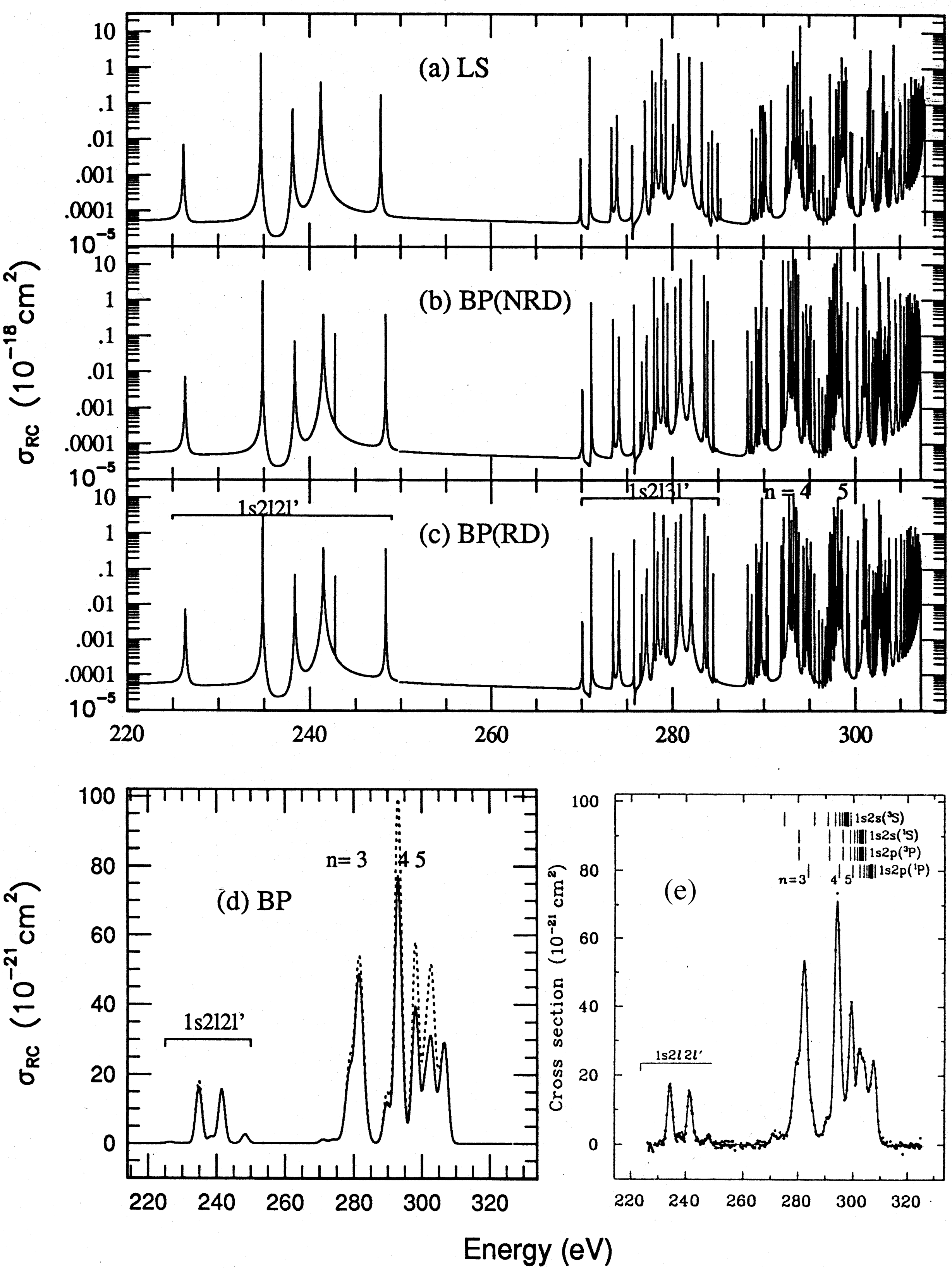
3 Results and Discussions

We have calculated the unified recombination cross sections of C V, C VI, and O VIII. Fig. 1 presents the detailed σ_{RC} for e + C V $\rightarrow$ C IV, obtained in three approximations, (a) in LS coupling and (b) in BP approximations, and (c) in the BP approximation with damping of low-*n* autoionizing states included. The (a) LS and the (b) BP(NRD) results are almost identical (except that the resonances are better resolved due to a much finer energy mesh in the BP case), indicating that the relativistic effects are negligible. The BP calculations involve considerably more recombination channels than the LS calculations because of nearly twice as many fine structure levels as LS terms, but the final results do not show a significant difference between the two. The difference is less between LS coupling and BP approximation when damping is included. The convoluted average of the two sets of BP results, with and without radiation damping, are shown in Fig. 1(d) - solid and dashed lines respectively. The BP(RD) results agree very well with experiment, Fig. 1(e).

The total $\alpha R(T)$ is obtained for all ions in the isonuclear sequence of oxygen, O I - VIII. Calculations, such as abundances and ionization fractions, require the rates for all ionization stages. The typical feature of $\alpha R(T)$ is similar to that of O IV as shown in Fig. 2 (solid curve) where, starting with high recombination at very low temperatures, $\alpha R(T)$ decreases to a minimum at $log_{10}(T)$ = 4.4 K for O IV, above which the DR dominates giving a "high T bump", such as the bump around $log_{10}(T)$ = 5.2 K for O VI, beyond which the rate falls smoothly with T. Due to near-threshold autoionization, a small bump may be observed in the low-T region. There is often considerable difference between the present and previously calculated values in the temperature region of interest such as shown in Fig. 2(b) where the sum of RR (dashed), low-T DR (dotted), and high-T DR (dot-dashed) rate curves [7] of Fig. 2(a) is compared with the present total recombination rate coefficients (solid) curve.

4 Conclusion

Unified electron-ion recombination cross sections, σ_{RC}, are obtained in the close coupling (CC) approximation. We find (i) very good agreement with the experiments, (ii) relativistic effects are small for the second row of elements, and (iii) radiation damping is significant for H-like and He-like ions only.



(a) LS
(b) BP(NRD)
(c) BP(RD)
1s2l2l'
1s2l3l'
n = 4 5
σ_{RC} (10^{-18}cm^2)
(d) BP
n= 3 4 5
1s2l2l'
σ_{RC} (10^{-21}cm^2)
(e)
1s2s(^{3}S)
1s2s(^{1}S)
1s2p(^{3}P)
1s2p(^{1}P)
n=3 4 5
1s2l2l'
Cross section (10^{-21} cm^2)
Energy (eV)

Figure 1

The total unified recombination rate coefficients, $\alpha R(T)$, for all oxygen ions, O I - O VIII, are obtained. So far $\alpha R(T)$ have been calculated for 30 other ions including all carbon ions, nitrogen ions, and carbon sequence ions C I, N II, O III, F IV, Ne V, Na VI, Mg VII, Al VIII, Si IX, and S XI, and Si I, Si II, S II, S III, and iron ions, Fe I - Fe V.

Acknowledgements

The work was partially supported by grants from NSF (Iron Project at OSU, PHY-9421898) and NASA. The computations were carried out on the Cray Y-MP at the Ohio Supercomputer center.

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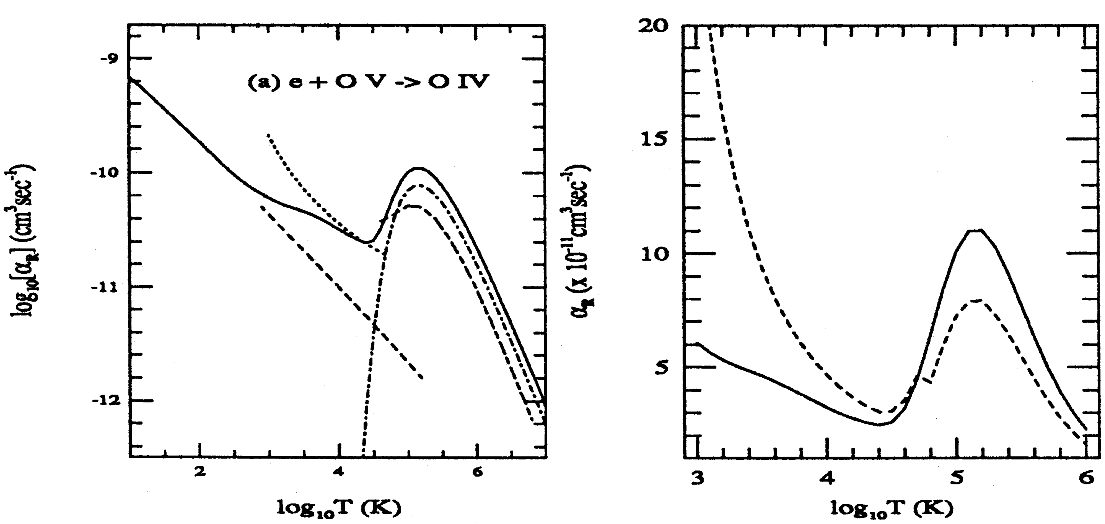

Figure 2