Relativistic Fine Structure and Resonance Effects in Electron-Ion Recombination and Excitation of (e + C IV)

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Relativistic close coupling calculations are reported for unified electronic recombination of (e + C IV) including nonresonant and resonant recombination processes, radiative, and dielectronic recombination (RR and DR). Detailed benchmarking of the theoretical unified results with two recent experiments on ion storage rings [S. Mannervik *et al.,* Phys. Rev. Lett. **81**, 313 (1998) and S. Schippers *et al.,* Astrophys. J. **555**, 1027 (2001)] shows very good agreement in the entire measured energy region $2s$-$2p$ with $2pn\ell$ resonances to ~15%. The resonant and the background cross sections are not an incoherent sum of separate RR and DR contributions. The electron impact excitation (EIE) cross sections are also compared with recent experimental measurements. Fine structure threshold effects in EIE and DR are delineated for the first time and should be of general importance.

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Although (e + ion) recombination has long been studied experimentally and theoretically, there appears to be considerable uncertainty over comparisons between measurements and theory, even for expectedly simple atomic systems such as C IV [1,2]. A comparison of the experimental (e + C IV) dielectronic recombination rates with theoretical data shows disagreement up to orders of magnitude [2]. However, as demonstrated by Mannervik *et al.* [1], using the ion storage ring CRYRING in Stockholm, there are complicated physical effects such as near-threshold fine structure resonances with unexpectedly large autoionization widths. Theoretically therefore, it is essential to account for both the relativistic and the complex electron correlation and resonance effects accurately. While experiments measure the combined cross sections for (e + ion) recombination, via the resonances and the background (since there is no natural separation between the two), they are still considered individually as dielectronic and radiative recombination (DR and RR). Apparently there are difficulties in measuring the nonresonant background at very low energies, possibly owing to external field effects [2]. But practical applications generally require (e + ion) rate coefficients, which in turn require cross sections for both RR and DR at all relevant energies. To that end a theoretical method has been developed for an *ab initio* unified treatment of both processes, based on the close coupling (CC) approximation and its relativistic extension, the Breit-Pauli R matrix (BPRM) method (e.g., [3–8]). The BPRM (e + ion) recombination cross sections for several ions have been compared with experiments, with excellent agreement in all cases [9]. It is therefore of interest to apply the BPRM method to elucidate the physical effects and issues related to (e + C IV) recombination, in direct comparison with experimental data [1,2]. Dielectronic recombination is also naturally linked to electron impact excitation (EIE). At the Rydberg series limit, as $n \to \infty$ (where the RR background is negligible), the photon flux in DR should, in principle, equal the electron scattering flux at threshold ($E = 0$), in accordance with unitarity [6,10]. Threshold fine structure would, however, give rise to a related structure in the DR and EIE cross sections.

In this Letter we present theoretical calculations based on the relativistic CC method to demonstrate that (i) the theoretical results for (e + ion) recombination agree with both ion storage ring measurements [1,2] to within experimental uncertainties, including near-threshold resonance strengths and nonresonant background, and (ii) fine structure resonance series and threshold effects in DR *below* the EIE threshold, which should be of general importance but have not heretofore been studied. The coupled-channel wave function expansion for an (e + C IV) may be expressed as

$$\Psi(E; e + \text{C IV}) = \sum_i \chi_i(\text{C IV})\theta_i(e) + \sum_j c_j \Phi_j(\text{C III}), \tag{1}$$

where Ψ denotes both the bound ($E < 0$) and the continuum ($E > 0$) states of C III, expanded in terms of the core ion eigenfunctions χ_i(C IV); the Φ_j are correlation functions. The CC approximation, using the efficient R-matrix method and its relativistic Breit-Pauli extension [12,13], enables a solution for the total Ψ, with a suitable expansion over the χ_i. The extension of the BPRM formulation to unified electronic recombination [6–8] entails the following. Resonant and nonresonant electronic recombination takes place in an infinite number of bound levels of the (e + ion) system. These are divided into two groups:

(*i*) the low-n ($n \leq n_0 \approx 10$) levels, considered via detailed CC calculations for photorecombination, with highly resolved delineation of autoionizing resonances, and (*ii*) the high-n ($n_0 \leq n \leq \infty$) recombining levels via DR, neglecting the background. In previous works (e.g., [6]) it was shown that in the energy region corresponding to (*ii*), below thresholds for DR, the nonresonant contribution is negligible. The DR cross sections converge to the electron impact excitation cross section at threshold ($n \longrightarrow \infty$), as required by unitarity, i.e., conservation of photon and electron fluxes. This theoretical limit is an important check on the calculations, and may also be used to show precisely the behavior of the resonances in DR fine structure cross sections as they approach and cross the fine structure thresholds towards the EIE cross section, as shown in this Letter.

The BPRM calculations for (e + C IV) recombination involve photorecombination into 212 low-n levels of C III, up to $\nu \leq 10.0$ (ν is the effective quantum number), and all SLJ symmetries with $J = 0-10$ (112 even parity levels and 110 odd parity levels). In the high-n energy region, $10 < \nu \leq \infty$, the background (RR-type) contribution to (e + ion) recombination is negligible. We calculate DR cross sections $\sigma_{\rm DR}$ due to the resonance series $^2P^0_{1/2}n\ell$, $^2P^0_{3/2}n\ell$ approaching the two fine structure thresholds $^2P^0_{1/2,3/2}$, and in between. Both the detailed $\sigma_{\rm DR}$ and the resonance averaged $\langle\sigma_{\rm DR}\rangle$ [6,10] are computed. Finally, the EIE cross sections $\sigma_{\rm EIE}$ are computed at the $^2P^0_{1/2,3/2}$ thresholds and above. Details of the calculations will be presented elsewhere, together with rate coefficients for practical applications.

Figure 1(a) shows the detailed unified (e + C IV) recombination cross section $\sigma_{\rm RC}$ in the $1s^22s(^2S_{1/2}) - -1s^22p(^2P^0_{1/2,3/2})$ region. In order to compare with experiment, we compute the rate coefficient $v \cdot \sigma_{\rm RC}$, and convolve with a Gaussian of ΔE (FWHM) that corresponds to the experimental resolution in the Test Storage Ring (TSR) [2]. Figure 1(b) shows the convolved theoretical results compared with the experimental results in Fig. 1(c) (Fig. 3 in [2]). The experimental results in Fig. 1(c) (solid dots) are reported in the region 2–8.5 eV, as shown, and compared with theoretical DR results (solid line) in [2] (multiplied by a factor of 0.8 and shifted by 0.06 eV). The present unified $\sigma_{\rm RC}$ in Fig. 1(a) show considerably more detail than the experimental results, but the convolved results agree remarkably well with the individual n complexes of resonances. We also incorporate an approximate field ionization cutoff in $\langle v \cdot \sigma_{\rm RC}\rangle$, experimentally estimated at $n_F = 19$, with the results shown as the dotted line in Fig. 1(b), compared to the dashed line in Fig. 1(c) [the dot-dashed line in Fig. 1(c) represents a model calculation of detection probabilities for high Rydberg states [2]]. A more accurate ionization cutoff may be possible by considering overlapping (n, J) manifolds of detailed $\sigma_{\rm RC}$ as in Fig. 1(a). At the series limit in Fig. 1(b) our results up to $n = \infty$ also agree very

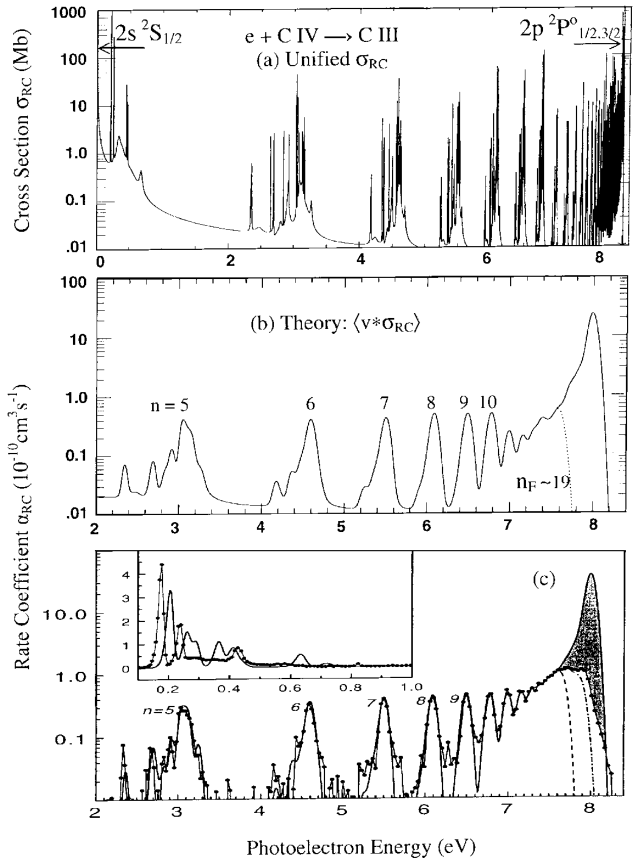

FIG. 1. (a) Unified (e + C IV) recombination cross section $\sigma_{\rm RC}$ with detailed resonance structures; (b) theoretical rate coefficient ($v \cdot \sigma_{\rm RC}$) convolved over a Gaussian with experimental FWHM [2]; (c) the experimentally measured rate coefficient [2]. The unified $\sigma_{\rm RC}$ in (a),(b) incorporate the background cross section eliminated from the experimental data in (c). The dashed and dot-dashed lines represent approximate field ionization cutoffs (see text).

well with the experimental results augmented as described in [2] [shaded portion in Fig. 1(c)].

Although the qualitative and the quantitative agreement in Fig. 1 appears to be excellent, the present unified results also include the background contribution, which was measured but subtracted from the reported experimental results. A very precise quantitative comparison can, however, be done for the resonance strength of the $2p4\ell$ complex measured by both the CRYRING [1] and the TSR [2] experiments. Figure 2(a) shows the present detailed unified $\sigma_{\rm RC}$ for the $2p4\ell$ complex, with the individual resonances identified. As in Fig. 1, the convolved $\langle v \cdot \sigma_{\rm RC}\rangle$ is shown in Fig. 2(b), and compared with (I) the CRYRING data (open circles), (II) TSR data (solid circles), and (III) calculated rate by Mannervik *et al.* [1] (shaded area) [Fig. 2(c)] that is up to 50% higher than the experimental values. We particularly note that our background rate $\alpha_{\rm RC} = 0.2 \times 10^{-10}$ cm^3 s^{-1} (solid circle) in Fig. 2(b), at $E = 0.1$ eV, agrees precisely with the measured background value reported in [2] at the same energy. Schippers

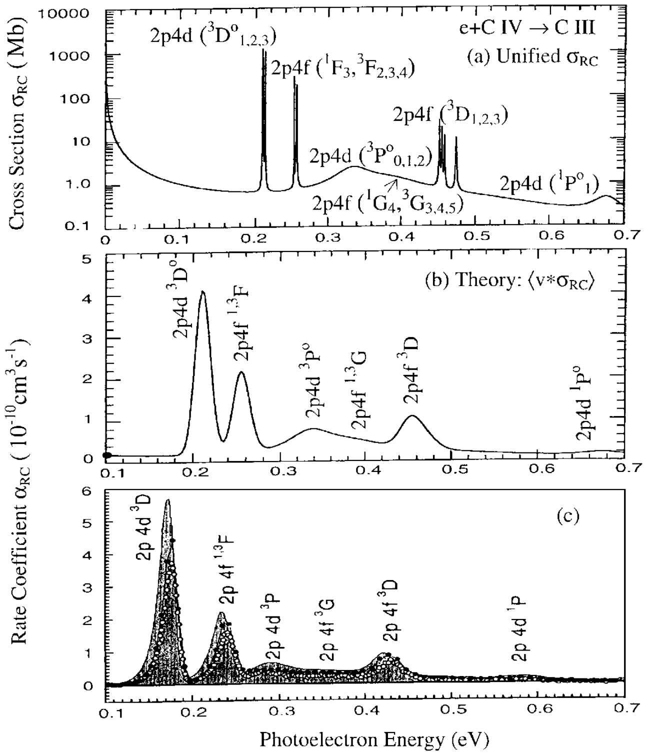

FIG. 2. (a) The $2p4\ell$ resonance complex, detailed unified $\sigma_{\rm RC}$; (b) convolved rate coefficient $(v \cdot \sigma_{\rm RC})$; (c) experimentally measured values from CRYRING [1] (open circles), TSR [2] (solid circles), and theoretical calculations from [1] (shaded region). The solid circle in (b) at $E = 0.1$ eV represents the experimentally measured background values (Fig. 7 in [2]).

et al. [2] quote the measured $2p4\ell$ resonance strengths of 1.9×10^{-11} eV cm^3 s^{-1} and 2.5×10^{-11} eV cm^3 s^{-1} from the CRYRING and the TSR data, respectively, a difference of about 30%. Our theoretical value is 2.16×10^{-11} eV cm^3 s^{-1}, obtained by direct integration over the resonances in Fig. 2(b), and subtracting a constant background of 0.2×10^{-10} cm^3 s^{-1} in the energy region covered by the resonances. Thus our theoretical value agrees better with each experiment, to $\sim$15%, than the two experimental values do with each other, differing by 30% (although each experiment has a reported uncertainty of 15%).

The present unified results confirm the experimentally measured background around $E \approx 0.1$ eV, as reported in Fig. 7 of [2], and in our Fig. 2(b). Whereas the experimental data are uncertain at very low energies, $E < 0.1$ eV, due to "excess recombination" possibly due to external fields, the background may not be as affected at higher energies $E > 0.1$ eV. We suggest that, except at energies close to the RR peak $E \approx 0$, the experiments accurately measure the total (e + ion) recombination cross sections that can, therefore, be directly compared with the unified theoretical calculations.

Schippers *et al.* [2] subtracted the background from the measured recombination cross sections to obtain the RR and DR contributions separately. They used near-hydrogenic approximations to estimate the additional RR contribution [14] to derive total recombination rates, which agreed with the earlier LS coupling rates of Nahar and Pradhan [15], to within experimental uncertainties at all temperatures except at low T, $<$5000 K [the discrepancy is due to the omission of K-shell excitation correlation functions Φ_j [Eq. (1)] that leads to some bound levels of C III appearing as resonances just at threshold]. However, as seen from Figs. 1 and 2, the (e + C IV) recombination cross sections may not be considered as an incoherent sum of RR and DR. The unified calculations, on the other hand, incorporate the background and resonant recombination in an *ab initio* manner, taking account of quantum mechanical interference between the RR and DR processes. We will compare these approximations in detail with the present more accurate BPRM photoionization calculations in the low-energy region in a subsequent paper on recombination rates for (e + C IV).

Next, we consider the threshold behavior of (e + C IV) DR and EIE. In Fig. 3 we delineate the fine structure $\sigma_{\rm DR}$ in the energy region spanned by the fine structure $^2P^0_{1/2,3/2}$ thresholds. Figure 3(a) shows the detailed resonances in the vicinity of the two series limits. Figure 3(b) shows the $\sigma_{\rm DR}$ averaged over the lower resonance series $^2P^0_{1/2}n\ell$

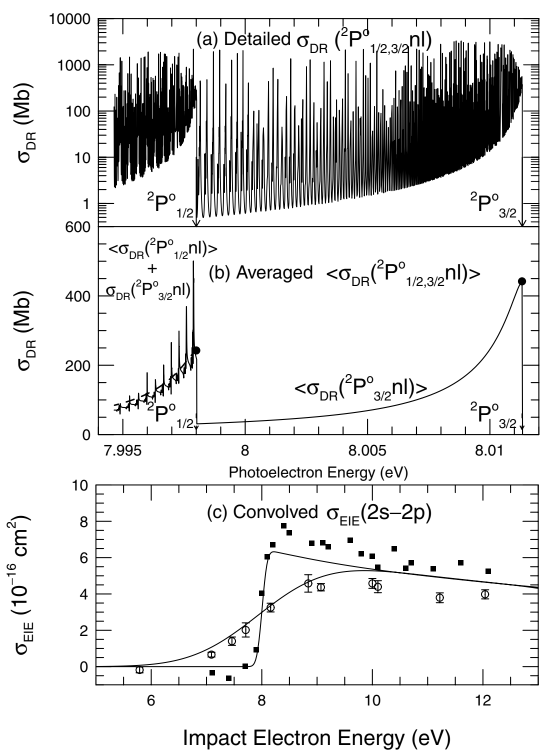

FIG. 3. $\sigma_{\rm DR}$ and $\sigma_{\rm EIE}$ of C IV: (a) detailed $\sigma_{\rm DR}$ with $^2P^0_{1/2,3/2}n\ell$ resonances; (b) $\sigma_{\rm DR}$ averaged over $^2P^0_{1/2}n\ell$ and detailed $^2P^0_{3/2}n\ell$ resonances (solid line), average over the $^2P^0_{3/2}n\ell$ (dashed line) (the solid circles are the peak averaged $\sigma_{\rm DR}$); (c) $\sigma_{\rm EIE}$ convolved over experimental data with FWHM = 0.175 eV from [16] (solid squares) and with FWHM = 2.3 eV from [17] (open circles).

below the $^2P^0_{1/2}$ level, but still with the detailed resonance structures due to the higher series $^2P^0_{3/2}n\ell$ (solid line). The $\sigma_{\rm DR}$ averaged over both series is shown as the dashed line. Above the $^2P^0_{1/2}$, $\sigma_{\rm DR}$ is averaged over the $^2P^0_{3/2}n\ell$ series. The sharp drop in the total $\sigma_{\rm DR}$ at the $^2P^0_{1/2}$ threshold reflects the termination of DR due to the $^2P^0_{1/2}n\ell$ resonance series, and with the $^2P^0_{3/2}n\ell$ contribution still low in spite of the fact that $n \approx 96$. The large drop in the DR cross section is due to enhanced autoionization in the excited level, when the $^2P^0_{1/2}n\ell$ channel opens up at the lower fine structure threshold $^2P^0_{1/2}$ while the radiative decay remains constant. The $\sigma_{\rm DR}(^2P^0_{3/2}n\ell)$ contribution builds up to the second peak at $^2P^0_{3/2}$.

In Fig. 3(b) it is shown that the resonance averaged $\lim_{n\to\infty}\langle\sigma_{\rm DR}(^2P^0_{1/2}n\ell)\rangle = 242.57$ Mb (dark circle at $^2P^0_{1/2}$), but the detailed $\sigma_{\rm DR}$ has resonances due to the higher series $(^2P^0_{3/2}n\ell)$ lying at and near threshold. The resonance averaged $\sigma_{\rm DR}$ at the next DR peak, $\lim_{n\to\infty}\langle\sigma_{\rm DR}(^2P^0_{3/2}n\ell)\rangle = 441.81$ Mb (dark circle at $^2P^0_{3/2}$). Interestingly, the fine structure in the theoretical $\sigma_{\rm DR}$ in Figs. 3(a) and 3(b) appears to be discernible as a small dip in experimental data in Fig. 2(c) just below 8 eV. Although the $^2P^0_{1/2,3/2}$ separation is only 0.013 eV, it may be possible to detect these fine structure threshold effects in future experiments with increased resolution.

At the $^2P^0_{1/2,3/2}$ thresholds the sum of the averaged fine structure $\langle\sigma_{\rm DR}\rangle = \sigma_{\rm EIE} = 684.38$ Mb. Figure 3(c) compares the near-threshold EIE cross sections with the absolute measurements from two recent experiments, (Greenwood *et al.* [16] and Janzen *et al.* [17]), convolved over their respective beamwidths of 0.175 eV [16] and 2.3 eV [17]. Our results are in good agreement with both sets (and also with another recent experiment by Bannister *et al.* [16,18]). Although the present results are the first CC calculations with relativistic fine structure for C IV, their sum is in good agreement with previous LS coupling CC calculations of $\sigma_{\rm EIE}$ [17,19,20].

In this Letter we demonstrate several new aspects of $(e$ + ion) recombination and excitation calculations and experiments: (*I*) the hitherto most detailed unified relativistic CC calculations agree with two sets of experimental data, such as to constrain both theoretical and experimental uncertainties to $\sim$15%, (*II*) except close to the RR peak at $E \approx 0$, the experiments perhaps need not eliminate the background entirely and may report the combined (RR + DR) rate in the future, (*III*) the finely delineated DR resonances could possibly be used to study field-ionization effects from the n, J-dependent partial DR cross sections, and (*IV*) the fine structure threshold effects in $(e$ + C IV) should manifest themselves more strongly in heavier and complex ions, in both DR and EIE.

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