Dielectronic recombination of O^+

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We have recalculated the dielectronic recombination rate coefficient for the special case of O^+ using an improved atomic structure. This removes the discrepancy between the results of Terao *et al.* [J. Phys. B **24**, L321 (1991)] and of Badnell and Pindzola [Phys. Rev. A **39**, 1690 (1989)].

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The process of dielectronic recombination (DR) has received a good deal of attention in the past few years, stimulated in the main by advances in experimental techniques, e.g., electron-beam ion traps and electron coolers. In general, there is good agreement between experiment and theory, and between the results of different theoretical groups. Recently, however, Terao *et al.* [1] calculated the DR rate coefficient for O^+ and found it to be nearly a factor of 2 smaller than that obtained by Badnell and Pindzola [2]. We will show that this is due to the inadequacy of the atomic structure used by the latter for the special case of O^+. Since the results of Terao *et al.* [1] were only obtained in *LS* coupling and since their original results [1] have subsequently been revised [1], we present here the results of a new intermediate-coupling calculation for the DR of O^+, which were obtained using an improved atomic structure. We also investigate correlation in the $(N+1)$-electron problem and the use of close-coupling (CC) versus distorted-wave (DW) threshold partial collision strengths to generate autoionization rates.

For the present calculations, we generated our atomic structure for O^+ using a modified version of the SUPERSTRUCTURE code [3]. We included the spectroscopic configurations, $2s^22p^3$, $2s2p^4$, $2p^5$, $2s^22p^23s$, $2s2p^33s$ and the correlation configurations, $2s2p^33\bar{d}$, $2s^22p^23\bar{d}$, $2s2p^33\bar{p}$ in our N-electron configuration-interaction (CI) expansion. Each spectroscopic orbital was generated using a single-configuration Hartree-exchange approximation [4]. Distinct local Hartree-exchange potentials for each orbital were generated using Slater-type orbitals, as described by Burgess, Mason, and Tully [5] for the case of the Hartree potential alone, and each contains an adjustable scaling parameter [5]. The correlation orbitals are screened hydrogenic functions. The scaling and screening parameters were determined by minimizing an equally weighted sum of the lowest three quartet terms. This gave an oscillator strength for the $2s-2p$ transition of 0.262, in good agreement with that obtained (0.268) from a more elaborate CI calculation by Bell *et al.* [6] and in close agreement with that used by Terao *et al.* [1]; also see Bell *et al.* [7]. We obtained 0.113 for the $2p$-$3s$ oscillator strength compared with a value of 0.139 obtained by Bell *et al.* [6]; the value obtained by Terao *et al.* [1] was about a factor of 2 smaller, but the $2p$-$3s$ core excitation only contributes about 10% to the total DR rate coefficient.

In their study of DR in the carbon and oxygen isonuclear sequences, Badnell and Pindzola [2,8] only allowed for $n=2$ correlation in the N-electron problem, for the $2s$-$2p$ core excitations, so as to keep the problem tractable. For the special case of O^+, there is no $n=2$ correlation, and it turns out that the $2s^22p^3\,{}^4S-2s2p^4\,{}^4P$ oscillator strength is particularly sensitive to $n=3$ correlation. Even though the length and velocity forms of the oscillator strength agree to better than 10% in a single-configuration calculation, they both overestimate the oscillator strength by nearly a factor of 2; see Ho and Henry [9] for a detailed discussion. As a result, the LS-coupling DR rate coefficient calculated using the more realistic atomic structure described above is substantially smaller than that of Badnell and Pindzola [2] and it is about 20% larger than the revised results of Terao *et al.* [1] for the $2s$-$2p$ core excitation.

The only remaining difference between the approach used here and that of Terao *et al.* [1] lies in the autoionization rates, since they also make use of the isolated-resonance and independent-processes approximations for DR. To investigate this, we have carried out 11-term CC and DW calculations of threshold partial collision strengths for O^+, using the same atomic structure (see above), making use of the "opacity"-coded version [10] of the R-matrix method [11] and the University College London–DW code [12]. By multiplying DW autoionization rates [13,14] by the ratio of CC to DW threshold partial collision strengths, we are able to evaluate the effect of continuum coupling on the DR rate coefficient for O^+. Including only those $(N+1)$-electron correlation configurations required by orthogonality, we find that the CC and DW threshold partial collision strengths differ by up to 30% for the $2s^22p^3\,{}^4S-2s2p^4\,{}^4P$ transition. However, the largest differences are for the low partial waves (S,P,D), which only contribute 30% to the total DR rate coefficient. This, together with the relative insensitivity of the DR rate coefficient to the autoionization rates, leads to a difference in the resulting DR rate coefficients of less than 1%.

Like the N-electron problem, the $(N+1)$-electron problem is also sensitive to correlation. We carried out another R-matrix calculation in which we included all possible $(N+1)$-electron configurations in the bound-state–bound-state part of the eigenfunction expansion

TABLE I. Intermediate-coupling dielectronic recombination rate coefficient for O^+ ($cm^3 s^{-1}$).

$\log_{10}[T\ (K)]$	σ_d (tot)
4.6	9.64 [−13][a]
4.8	2.60 [−12]
5.0	3.87 [−12]
5.1	4.05 [−12]
5.2	3.92 [−12]
5.4	3.09 [−12]
5.6	2.07 [−12]
5.8	1.25 [−12]
6.0	7.01 [−13]
6.2	3.78 [−13]
6.4	1.99 [−13]
6.6	1.03 [−13]

[a] $9.64[-13] = 9.64\times10^{-13}$.

[11]. This approach can lead to problems due to missing continua [15] and/or pseudoresonances [16], but, by focusing on excitation energies below the lowest missing continuum states and by avoiding pseudoresonances [their positions can be determined from an $(N+1)$-electron structure calculation using the bound orbitals from the N-electron problem] we were able to generate reliable results in the energy region of interest. Although this calculation only reduced the total threshold collision strength by about 20%, there were some much larger differences on individual low partial waves (e.g., a factor of 6 on $^5D^\circ$). When we used these partial collision strengths in the DR problem, we found that the total rate coefficient was reduced by 10%. Thus, a more elaborate treatment of correlation in the $(N+1)$-electron problem (e.g., Ref. [1], [6], or [7]) is unlikely to have a significant effect on the total DR rate coefficient for O^+. Indeed, our LS-coupling results for the $2s$-$2p$ core excitation now differ by less than 10% from the revised results of Terao *et al.* [1].

Previously, we found that intermediate coupling increased the DR rate coefficient for O^+ by nearly 25% [2]. We find that the same remains true on using the improved atomic structure and CC correction factors for the autoionization rates. We present our final results in Table I. In fact, the general conclusions of Badnell and Pindzola [2] and of Krylstedt, Pindzola, and Badnell [17] that were based on relative results for O^+ remain largely unchanged, e.g., the effect of alternative Auger channels, intermediate coupling, electric fields, and the accuracy of the Burgess general formula [18]. Only the absolute results have changed, the present total DR rate coefficient for the high-temperature peak in O^+ being 35% smaller than the original intermediate-coupling result of Badnell and Pindzola [2]. Furthermore, their [2,8] oscillator strengths for the transitions that dominate the DR of the remaining C and O ions are accurate to 15% or better, based on comparisons with the results of more elaborate calculations; see, e.g., Yan, Taylor, and Seaton [19], Luo *et al.* [20], and Aggarwal and Hibbert [21].

In conclusion, we have shown the importance of allowing for correlation in the N-electron problem (e.g., radiative rates) in the determination of an accurate DR rate coefficient for O^+. However, the use of a simple perturbation-theory expression for the autoionization rates, which neglects continuum coupling and $(N+1)$-electron correlation effects, does not lead to a significant error in the DR rate coefficient despite the nontrivial nature of these effects on autoionization. In general, increased sensitivity of DR to the autoionization rates only occurs with increased residual charge, for which continuum coupling and correlation effects are substantially reduced.

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