Fine structure and resonance transitions in C^+

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Certain significant features in the collision strengths for electron-impact excitation of the fine-structure transition $^2P^\circ_{1/2}$-$^2P^\circ_{3/2}$ and the resonance transition $^2P^\circ$-^2D in C^+ are discussed based on improved calculations.

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I. INTRODUCTION

R-matrix calculations in the close-coupling approximation have been reported earlier by Luo and Pradhan [1] for electron-impact excitation of a number of transitions in C^+, N^{2+}, and O^{3+} including fine structure. Of particular interest is the fine-structure transition within the ground state, $^2P^\circ_{1/2}$-$^2P^\circ_{3/2}$, and the first dipole-allowed (resonance) transition $^2P^\circ$-^2D. The former transition gives rise to a well-known [2,3] line in the infrared spectra of many astrophysical sources and it is important to determine the excitation cross section and rate coefficient accurately. The resonance transition in C^+ is currently the subject of experimental investigations using the crossed-beam [4] and the merged-beam techniques [5] for electron-ion scattering. Owing to the importance of these transitions we have entirely repeated the calculations of Luo and Pradhan, improving upon them in a number of respects.

The fine-structure transition $^2P^\circ_{1/2}$-$^2P^\circ_{3/2}$ has been considered by a number of previous studies, both in electron-C^+ scattering [2,3] and photoionization calculations [6,7] for C°. The cross sections are seen to be dominated by an autoionizing state, $2s2p^3(^1D^\circ)$, that lies just above the excitation threshold. Two of the previous calculations, by Luo and Pradhan [1] and Lennon *et al.* [3], obtained the resonance shape and position in substantial agreement with each other, and in disagreement with that of Hayes and Nussbaumer [2]. Although the $2s2p^3(^1D^\circ)$ level has not been observed, it was suggested by both Lennon *et al.* and Hayes and Nussbaumer that in calculating the rate coefficients the resonance position should be shifted closer to the excitation threshold to coincide with the value predicted by Edlen [8] in 1934. In the present study we extend the work of Luo and Pradhan to analyze the $^2P^\circ_{1/2}$-$^2P^\circ_{3/2}$ collision strength in terms of the individual angular momentum contributions with respect to the position and the shape of the resonance structures.

For the dipole transition, $^2P^\circ$-^2D, the work of Luo and Pradhan is also extended to include more partial waves explicitly in the close-coupling calculations and collision strengths in the region above all excitation thresholds are obtained (the earlier work did not consider this region due to the presence of pseudoresonances).

II. CALCULATIONS

Some of the improvements made over the previous Luo and Pradhan calculations are as follows.

(i) Observed target energies were substituted for calculated ones in the eigenfunction expansion, thus giving a more precise scale for the positions of autoionizing resonances. The ten target states included in the calculations are as follows: $2s^22p(^2P^\circ)$, $2s2p^2(^4P,^2D,^2S,^2P)$, $2s^23s(^2S)$, $2s^23p(^2P^\circ)$, $2p^3(^4S^\circ,^2D^\circ,^2P^\circ)$. Although the experimental and the calculated target energies are very close with the maximum discrepancy of 3% for the ^4P state [1], the small corrections to the eigenvalues of the diagonal elements of the Hamiltonian for the target ion give a slightly better representation of the positions of the Rydberg series of resonances that might affect the calculation of Maxwellian averaged rate coefficients. Given the extensive resonance structures present, and the sensitivity of the rate coefficients to these, the present calculations should yield better accuracy.

(ii) A more complete partial-wave expansion is employed for enhanced accuracy in the collision strengths for dipole-allowed transition; in the present work we employ partial waves up to $l \leq 10$, whereas the earlier work used $l \leq 4$, along with a Coulomb-Bethe-type method for "topping-up" or completing the partial-wave summation. Also, in the present work we have obviated the problem of pseudoresonances, in the region of all channels open, which did not enable the previous work to obtain accurate collision strengths in this region. The close-coupling calculations for $l \leq 10$ are carried up to the highest threshold of excitation of C^+ (with the top-up procedure as before). However, in the region of all channels open, we carry out separate Coulomb-Bethe calculations and *normalize* the results at the highest threshold, $2p^3(^2P^\circ)$, to the ten-state close-coupling (hereafter 10CC) calculations. It is known that the Coulomb-Bethe (hereafter CBe) approximation overestimates the collision strengths due to low partial waves describing close encounters [9]. This, for example, was found to be the case for all dipole transitions considered in the present work. The normalized results are labeled as 10CC+CBe and show a smooth variation with energy, consistent with the theoretical Bethe form $\Omega \sim \ln E$, free of pseudoresonances

that appear in many close-coupling calculations (due to correlation-type functions often represented by pseudo-orbitals [10]).

(iii) The calculations of Luo and Pradhan [1] were carried out using the R-matrix package of codes developed for the Opacity Project [11]. The fine-structure collision strengths were calculated using a new code, STGFJ, that separately transformed the reactance matrices obtained from the R-matrix codes from LS to a pair-coupling representation.

Some errors in the earlier work have been corrected. Although these are minor, mostly related to incomplete summation over some contributing channels of high-symmetry states ($J\pi$) in pair coupling, the final results for some of the transitions are affected; the $^2P^\circ_{1/2}$-$^2P^\circ_{3/2}$ collision strength changes by a few percent over the energy range considered. The procedure has also been improved by incorporating STGFJ directly into the R-matrix package of codes [11], thus enabling more detailed calculations to be carried out in a flexible manner, in particular by varying energy meshes and by delineating the individual contributions from the various total $J\pi$ states to the fine-structure collision strengths.

III. DISCUSSION OF RESULTS

A. Ground-state fine-structure transition

In Fig. 1 we present the total and the individual $J\pi$ contributions to the collision strength for the fine-structure transition $^2P^\circ_{1/2}$-$^2P^\circ_{3/2}$. It has been pointed out by Keenan *et al.* [12] that the collision strength exhibits a near-threshold resonance, due to the autoionizing state $2s2p^3(^1D^\circ)$, with a broad shoulder on the low-energy side. The calculations by Hayes and Nussbaumer [3], on the other hand, showed the shoulder to be on the high-energy side. Our results, and the results of Keenan *et al.*, show that the low-energy rise is due to the contribution to the collision strength by the total $J\pi$ symmetry $J=2$, odd parity. Our further analysis for other $J\pi$ symmetries, $J=0,1,2,3$ even and odd parities, shows all of those to contribute in the higher-energy region.

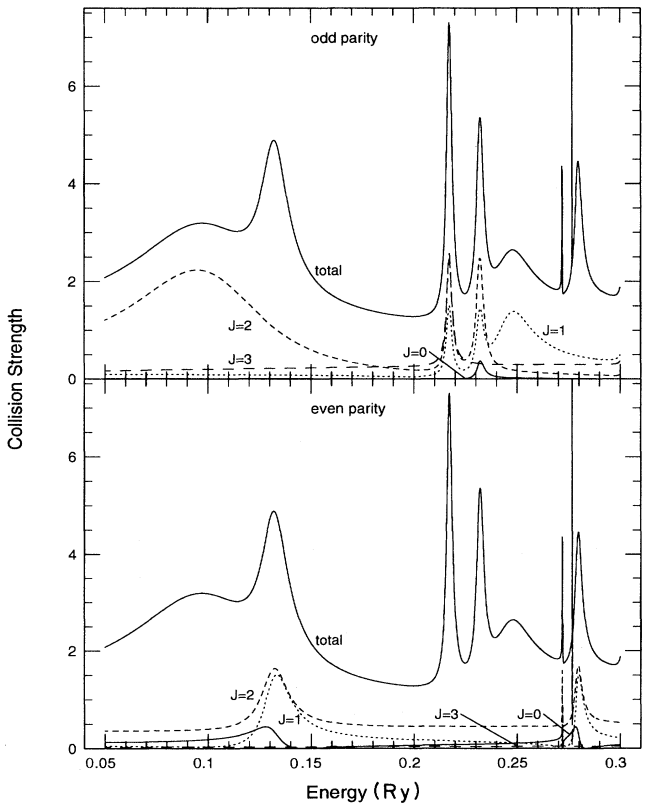

FIG. 1. Individual and total $J\pi$ contributions to the collision strength for the $2s^22p(^2P^\circ_{1/2}$-$^2P^\circ_{3/2})$ fine-structure transition.

It is important to determine, as precisely as possible, the detailed shape and position of this resonance as it influences the Maxwellian averaged rate coefficient for this transition to a great degree. The present results in Fig. 1 show the resonance to be at an energy somewhat lower than that of Keenan *et al.*, but essentially confirming the position and the shape that they obtain, and in disagreement with that of Hayes and Nussbaumer. However, both the previous calculations recommended that the calculated position of this resonance should be shifted by -0.06 Ry to coincide with the apparently observed position by Edlen (1934) [8]. An investigation of the work by Edlen shows that the position of the $2s2p^3(^1D^\circ)$ resonance was not in fact observed but rather extrapolated from the observed positions of the *bound* state in N^+ and O^{2+}. As such, the extrapolated position may not be highly reliable [13].

Nussbaumer and Storey [14] have carried out extensive configuration-interaction-type bound-state calculations for a large number of bound states of C°, including low-lying autoionizing states, to obtain recombination rate coefficients. However, for the $2s2p^3(^1D^\circ)$ state they quote only the extrapolated value by Edlen. In an effort to determine the position from bound-state atomic structure calculations we employed the SUPERSTRUCTURE program [15] with an even more extended basis set than Nussbaumer and Storey consisting of 66 configurations. However, the resulting value was much higher, 0.15 Ry above the C^+ ionization threshold, than the close-coupling calculations which yield the resonance position to be at 0.09 Ry. The photoionization calculations by Burke and Taylor [6] and Hofmann, Saha, and Trefftz [7] also report higher values, 0.12 and 0.14 Ry, respectively. In any case, a detailed comparison by Luo and Pradhan [16] with the work of Nussbaumer and Storey and other workers shows that the close-coupling results for the bound states of C° and N^+ are at least as accurate as the large configuration-interaction-type calculations. This is also reflected in the close agreement with experiment for the radiative transition probabilities for all transitions considered, a reliable indicator of the accuracy of the wave functions calculated [16]. We therefore suggest that the present resonance position and the collision strength in the near-threshold region is accurate and may not require a shift to lower energies.

The precise effect on the rate coefficients is shown in Table I, where the two sets of values under "Keenan *et al.*" are the Maxwellian averaged collision strengths by Keenan *et al.* with and without the shift of the

TABLE I. Maxwellian averaged collision strengths for the $2s^2 2p\,(^2P^o_{1/2}\text{-}^2P^o_{3/2})$ transition. The two columns under "Keenan *et al.*" are the rate coefficients by Keenan *et al.* with and without the shift of the $2s2p^3(^1D^o)$ resonance to the lower energy.

	Keenan *et al.* [12]		
$\log_{10}T$ (K)	Without shift	With shift	Present
3.0	1.60	2.16	1.58
4.0	2.11	2.76	2.15

$2s2p^3(^1D^o)$ resonance to the lower energy, compared with the present values at two temperatures that mark the range of interest in practical applications. While we reconfirm the unshifted values of Keenan *et al.*, the maximum difference between the two sets of rate coefficients is approximately 30% at the temperature of 1000 K. It is possible that with the lower value for electron-impact excitation some other process may be more important in the excitation of the ground-state fine-structure transition, e.g., H impact on C^+. Perhaps the final resolution of the discrepancy appears to be an experimental reexamination of the resonance position; we hope that the present work will provide an incentive for such a study.

B. Resonance transition

The collision strength for the $^2P^o\text{-}^2D$ transition is presented in Fig. 2, showing the combined 10CC+CBe calculations. The present results are slightly higher than those of Luo and Pradhan [1] at threshold. The rich resonance structure in the region covered by the ten states included in the eigenfunction expansion has been delineated and shows a significant enhancement in the energy range 0.8–0.9 Ry (the excitation threshold energy is 0.6824 Ry). The enhancement, relative to the background, appears to be sufficiently large to be observed experimentally. The present collision strengths, with more partial waves included, are 5–10 % higher than the values of Luo and Pradhan [1] in the energy range considered.

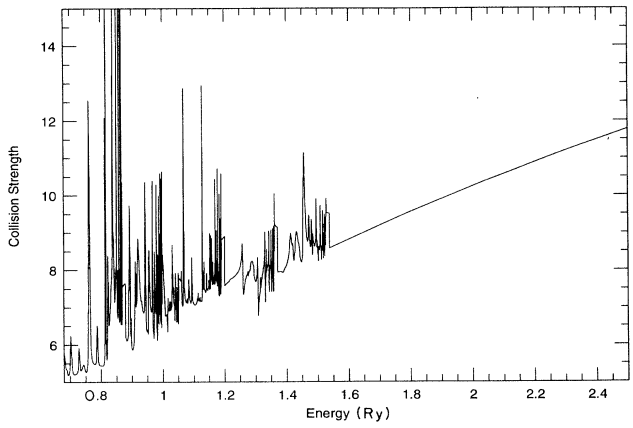

FIG. 2. Collision strength for the $^2P^o\text{-}^2D$ resonance transition showing the combined 10CC+CBe results, where the CBe value is matched to the CC value at the highest target threshold in the CC expansion.

At the energy of the highest threshold, $2p^3(^2P^o)$, the CBe collision strengths were scaled uniformly to the 10CC collision strengths (including the high-l top-up), by an amount equal to the difference between the 10CC and the CBe values *at only this energy*. No other adjustment was made to the CBe values. A very satisfactory energy behavior appears to have been thus obtained as one can readily discern that the *background* collision strength, from the excitation threshold onwards, shows a fairly smooth and monotonic increase all throughout the energy range characteristic of an optically allowed transition. This relatively simple method appears to effectively treat the high-energy region where pseudoresonances often plague the otherwise highly accurate close-coupling calculations. Of course in this particular case the energy range above the $2s2p^3(^2P^o)$ threshold is not likely to affect the rate coefficient for this transition as the Maxwellian at typical temperatures of around 10 000 K for the abundance of C^+ assumes extremely small values.

C. Comparison of *LS* multiplet to fine-structure collision strengths

The collision strengths for fine-structure transitions are calculated through an algebraic transformation of the reactance matrices (i.e., the K matrices) to a pair-

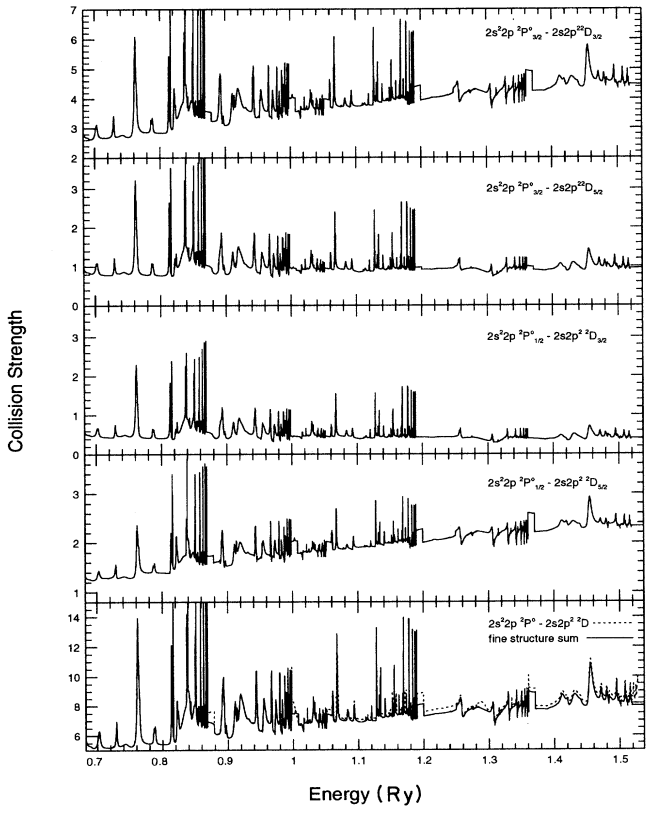

FIG. 3. Comparison of the *LS* multiplet and the sum of the fine-structure collision strengths for the $^2P^o\text{-}^2D$ transition. The individual fine-structure components of the *LS* multiplet collision strength are also shown.

coupling representation. While the collision strengths for the multiplet transitions in LS coupling enable a top-up procedure to be employed based on the CBe approximation [17], no such procedure has been developed for the fine-structure transitions. Furthermore, the fine-structure collision strengths are calculated by transforming the K matrices for all the contributing total $SL\pi$ symmetries to the total $J\pi$ states for the e +ion system and the two sets of total symmetries (in LS and pair-coupling representations) do not precisely match in terms of individual contributions. Therefore in order to ensure that the fine-structure collision strengths are complete, particularly for the allowed transitions where a relatively large number of partial waves may contribute, it is necessary to include a sufficient number of $SL\pi$ states in the LS coupling calculations to attain convergence.

A useful check on the individual fine-structure collision strengths is provided by comparing the *sum* of the fine-structure components with the LS coupling values for the whole multiplet, i.e., $\sum_{J_i,J_{i'}} \Omega(S_iL_iJ_i - S_{i'}L_{i'}J_{i'})$ with $\Omega(S_iL_i - S_{i'}L_{i'})$. In Fig. 3 we show the collision strengths for the fine-structure components $^2P^o_J$-$^2D_{J'}$ of the $^2P^o$-^2D multiplet and compare with the total. The close agreement between the two is an indication of the fact that the fine-structure collision strengths have converged in the same way as the total multiplet collision strength in terms of the contributing partial waves. Owing to some errors in the work of Luo and Pradhan [1], the individual fine-structure collision strengths did not add up to the total LS values, although the discrepancies were no more than 20% in the worst case.

In addition to the theoretical requirement that the sum of fine-structure components should add up to the LS value if only an algebraic transformation is carried out, it is also of practical importance in that we can now determine the rate coefficients for the individual components for the optically allowed fine-structure transitions; this has not been done before to our knowledge. Often the observed spectra consist of lines corresponding to the transitions within the fine-structure components rather than the whole multiplet. This is increasingly the case as the resolution of the spectroscopic instruments improves.

Further extending the work of Luo and Pradhan, rate coefficients have been computed for a large number of transitions, including all the fine-structure sublevels, at a range of temperatures for C^+, N^{2+}, and O^{3+}. The data involve 153 transitions in C^+ and 105 transitions in N^{2+} and O^{3+} corresponding to 18 and 15 states, including fine structure, respectively. Rate coefficients for each transition are planned to be tabulated at approximately ten temperatures close to the maximum abundance of each ion in ionization equilibrium [18].

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