Excitation of C^{3+} by electron impact

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The $2s$-$2p$ transition in the lithiumlike ion C^{3+} is studied in the resonance region below the $n = 3$ threshold. A five-state close-coupling expansion is used. Cross sections are calculated using the R-matrix method for $0 \leq L \leq 4$ and the noniterative integral-equation method for $L > 4$. A complicated structure of numerous, generally narrow, resonances is obtained for impact energies in the range 1.4–2.6 Ry. The resonances lead to a small overall enhancement of the average cross section.

INTRODUCTION

Lithiumlike ions can be important in both controlled thermonuclear and astrophysical plasmas.[1-3] There have been several previous studies of excitation processes in such ions; references to work prior to 1975 can be found in reviews by Bely and van Regemorter[4] and by Seaton.[5] In addition, we note more recent studies of van Wyngaarden and Henry,[6,7] and Gau and Henry.[8] However, the work cited concerns either the energy region above the ionization threshold, or involves approximations (such as Coulomb-Born and its variants, and two-state close coupling) which can not describe resonances in excitation cross sections.

It is well known that infinite series of resonances lie under each of the excitation cross sections in positive ions.[5] The existence of such resonances introduces uncertainty as to the validity of approximate calculations of excitation rates (and thus of plasma properties) in which the effects of closed channels are ignored. It is, however, a lengthy and complicated process to analyze the possible resonant structure of even a relatively simple system such as a lithiumlike ion unless a purely analytic treatment is employed.[9] The purpose of the present paper is to report a detailed study of the effect of resonances under the $n = 3$ thresholds on the $2s \rightarrow 2p$ excitation cross section in C^{3+}. This is the first calculation of this sort for a lithium like ion of which we are aware.

We obtain a complicated structure of narrow, highly asymmetric resonances for incident energies in the range 1.4–2.6 Ry. The most important are associated with the $^1P^o$, ^1D, ^3D, and ^1G states of the compound, four-electron system. An average over these resonances leads to a small enhancement (3%) of the overall excitation cross section.

PROCEDURE

The $2p$ state of C^{3+} is 0.59 Ry above the $2s$ state while the excitation energies of the $3s$, $3p$, and $3d$ states are 2.76, 2.92, and 2.97 Ry respectively. The lowest resonance above the $2p$ states occurs at about 1.48 Ry. We have investigated $2p$ excitation from an energy of 1.40 Ry, below the lowest resonance, to 2.6 Ry. Above 2.6 Ry, the structure becomes so narrow and so closely spaced that it would be extremely time consuming to resolve the resonances in detail. In addition, we have limited our studies of resonances to the lowest five partial waves, S through G. The lowest resonances of interest to us are (roughly) associated with temporary bound states $(3l, 3l'; l, l' = 0, 1, 2)$. The largest total angular momentum that can be formed in this way is $L = 4$. Thus, inclusion of $0 \leq L \leq 4$ is sufficient to yield the lowest, and presumably most important resonances. The first resonance which will not be included in our cross section study is $^3H^o$, which we estimate will occur close to 2.32 Ry.

Our studies of resonance effects are based on a five state close coupling approximation ($2s$, $2p$, $3s$, $3p$, and $3d$) with exchange. The $(1s)^2$ core is treated as frozen. This approach has been widely employed in studies of Li-like ions. The coupled integro-differential equations, to which the close coupling expansions lead, are solved by the R-matrix method,[10] using a program developed by Berrington *et al.*[11] The ionic wave functions used in the expansion are Hartree-Fock wave functions given by Weiss.[12] This procedure has been used to obtain partial cross sections for about 150 values of the incident electron energy in each of the ten (angular momentum and spin) states from ^1S through ^3G.

Examination of the results of these calculations reveal a bewildering amount of structure. For

example, we find 14 resonances in the $^1P^o$ state between 1.4 and 2.6 Ry. While some of the lower resonances have widths of the order of 0.01 Ry, most are considerably narrower with widths of the order of a few times 0.001 Ry.

Our first concern is to verify that the resonances obtained are genuine. To this end, we make some straightforward calculations by the stabilization method,[13] looking for two-electron excited (autoionizing) states of C^{2+}. This is done, with the $(1s^2)$ core frozen, by expanding the wave function for the outer two electrons as a symmetrized sum of pairs of orbitals with the required L, S and parity $[(-1)^L]$. We use orbital bases containing up to 44 terms (for example 15s orbitals, 10p, 7d, 6f, 5g, and 1h). Stabilized eigenvalues are found corresponding to most of the structures in the cross section below 2.4 Ry. A few instances of structure in the cross section are uncovered which did not have nearby stabilized eigenvalues. More detailed investigation reveals that these cases correspond to regions of rapid variation in the eigenphases where, however, no eigenphase passed through $\pi/2$. Comparison calculations were made with a different method discussed subsequently and did not show structure. Evidently the R-matrix method can yield spurious resonances in some circumstances. Subsequent investigation showed that this structure is an artifact resulting from incomplete cancellation of large numbers in evaluating the Buttle correction (see Ref. 10). We have simply deleted results at energies where this structure occurred.

We have developed the following procedure to analyze our results, based on the work of Eissner and Seaton.[14] Let E_R be the energy of a resonance in some channel (specified by $L, S, \Pi, \ldots$, etc.) Then near E_R, each element of the reaction matrix K has the form

$$K_{ij} = K_{ij}^{(0)} + C_{ij}/(E_R - E), \tag{1}$$

where the nonresonant background is represented by the slowly varying quantity $K_{ij}^{(0)}$. Seaton shows further that the residues C_{ij} can be factored:

$$C_{ij} = c_i c_j . \tag{2}$$

In order to fit our calculated K matrices, we adopt the representation

$$K_{ij}(E) = \sum_{n=0}^{N} D_{ij}^{(n)} (E - E_o)^n + \sum_{\lambda} \frac{C_{ij}^{(\lambda)}}{E_\lambda - E} . \tag{3}$$

The first term on the right describes the background: it is assumed to be representable as a polynomial. The quantity E_o is the (arbitrarily chosen) lowest energy at which the fit is made. The number of terms included in the first summation is adjusted to give a fit of satisfactory accuracy. The second sum in (3) represents the contribution from all the resonances in the energy region considered.

In practice, it is relatively easy to obtain rather accurate values for the energies of the resonances. Close to a specific resonance, Eq. (1) applies. Then from the values of any element of K at three points in the neighborhood of the resonance, E_R is determined. Alternately, one may use the tangent of an eigenphase. When the E_λ have been determined, one has a set of linear equations for the remaining unknowns. The coefficients are independent of the particular element K_{ij}, and it is both simple and quite satisfactory to apply the least-squares method to determine them. We are able to reproduce the initial K matrix at each point with a typical accuracy of 1% or better.

Once the coefficients C and D in Eq. (3) have been determined, the K matrix, and hence the cross sections can be easily determined at as many energies as are desired. In particular, cross sections may be generated on a fine enough mesh of points to permit numerical integration.

As mentioned earlier, the R matrix method is used only for values of the total angular momemtum L, $0 < L < 4$. The contribution from larger values ($5 \leq L \leq 9$) is obtained using a noniterative integral equation method (NIEM),[15,16] applied to the five-state expansion (including exchange). The same method is used to examine regions of energy for smaller values of L at energies where the R-matrix method is believed to produce spurious structure and it confirms our conclusions based on the stabilization calculations. For angular momenta in the range $10 \leq L \leq 15$, the Coulomb-Born approximation was employed, and for $L \geq 16$, the Coulomb-Bethe approximation. The results from these approximations join smoothly.

Calculations for the higher angular momenta were made for incident energies of 1.4, 1.8, and 2.2 Ry, all of which lie below the lowest resonance under the $n = 3$ thresholds for $L \geq 5$. The results were fit with a quadratic formula in order to interpolate for energies intermediate between 1.4 and 2.2. For higher energies, the results were simply extrapolated using the same formula. This process ignores all resonances for large L and certainly introduces some error which we are not able to assess.

RESULTS

The partial cross sections for excitation show pronounced resonant structure. Three examples are shown: $^1P^o$ (Fig. 1), ^1D (Fig. 2), and ^1G (Fig. 3). These states exhibit the broadest and most important resonances; however, resonances are found for all the partial waves investigated. The positions of all the resonances we have found

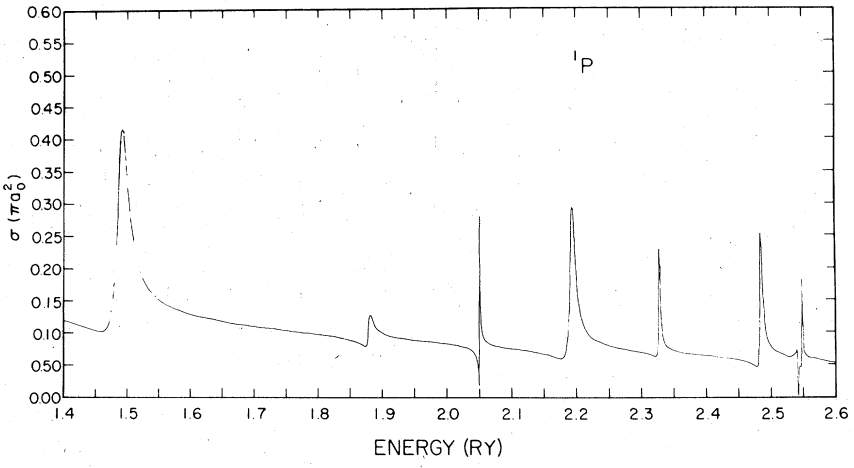

FIG. 1. A partial cross section in units of πa_0^2 for the $2s \rightarrow 2p$ excitation of C^{3+} in the state $^1P^o$ is shown as a function of the energy of the incident electron from 1.4 to 2.6 Ry.

in the range 1.4–2.6 Ry (above the ground state) using the R-matrix program are given in Table I. It is, of course, possible that some extremely narrow resonances have been overlooked. The resonances correspond to autoionization states of the ion C^{2+}, and it is possible that some of these (the $^1P^o$ series) might be observed in photoexcitation experiments. The scattering calculation from the ground state of the ion involves only those states whose parity is $(-1)^L$ (L is the total angular momentum), and we have no results for resonances of opposite parity.

The resonances of each series have rather characteristic shapes, some of which are reasonably approximated by the standard formula

$$\sigma = \sigma_B + \frac{B(\Gamma/2) + A(E - E_R)}{(E - E_R)^2 + \Gamma^2/4}. \qquad (4)$$

However, several of the resonances can be fit only rather poorly by this expression. For this reason, the determination of a meaningful width parameter, Γ, is not as simple as one might anticipate. We have made least-squares fits to the cross sections in the vicinity of the low-energy resonances using Eq. (4) and have also estimated Γ from the behavior of the eigenphases. Our results for widths are given in Table II. It would not be meaningful to present more significant figures than we have shown. Some general conclusions can be drawn: The widths of resonances in the triplet states tend to be considerably smaller than those in the singlets. The widths of the lower resonances tend to be greater than those of the higher ones, but the decrease is not uniform with energy.

We are unable to make a specific assignment of

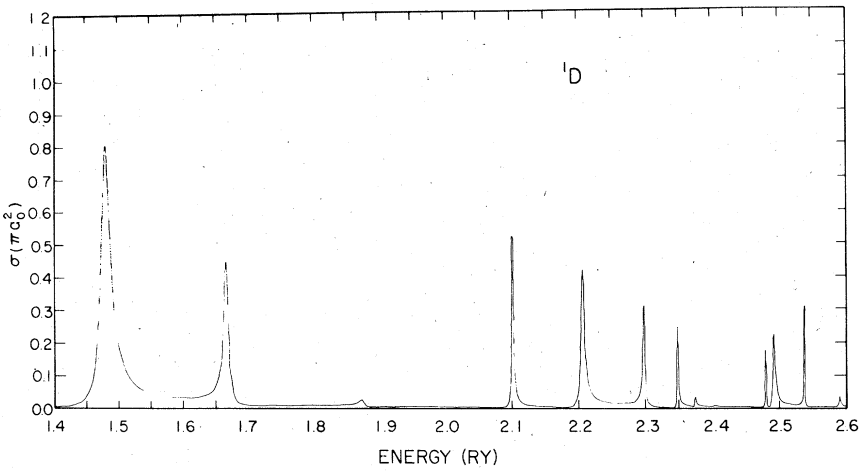

FIG. 2. Similar to Fig. 1 for the D^1 state. Note difference in the vertical scale.

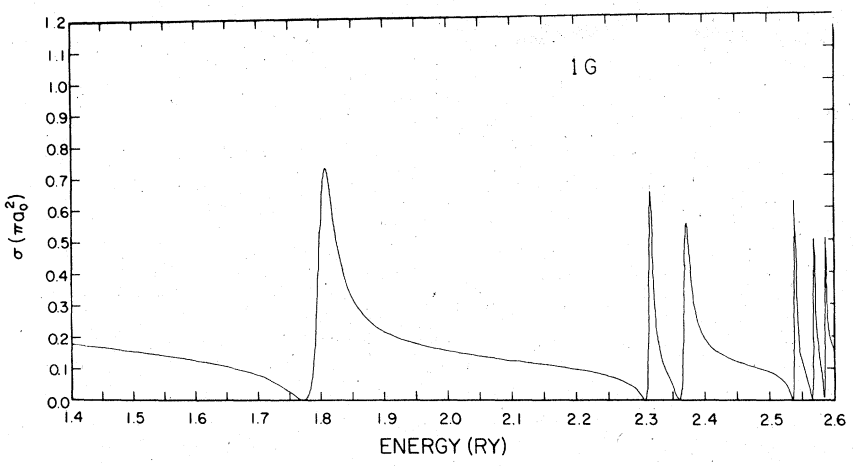

FIG. 3. Similar to Fig. 1 for the ^1G state. Note difference in the vertical scale.

dominant configuration in most cases. Difficulties arise because of configuration interaction. For example, the nearly degenerate configurations $3s$-$3d$, $3p^2$, $3d^2$ can form ^1D. Presumably the lowest three ^1D resonances are combinations of these. There are a few special cases where a single configuration can plausibly be assigned. The lowest ^3D resonance should be $3s$-$3d$. The lowest ^1G must be mostly $(3d)^2$, but the next higher ones can mix $3d$-$4d$ with $3p$-$4f$. The lowest $^1F^o$ (and $^3F^o$) should be $3p$-$3d$. As the principal quantum number of the outer electron increases, more and more nearly degenerate configurations can interact to form the actual resonant state.

The total excitation cross section for excitation is shown in Fig. 4, including the contribution from states $L \geq 5$ as previously discussed.[17] The complicated structure of resonances is obvious. Vertical bars identify the positions of the more important resonances which contribute to the structure.

The total cross section for the $2s \rightarrow 2p$ transition in C^{3+} has been measured by Taylor *et al.*, however only a preliminary report is available.[18] The narrowness of many of the resonances, as well as the large nonresonant background coming from high L partial waves, may make observation of the structure we predict difficult. To indicate what may be realistically expected from an experiment, we have averaged the calculated cross section with a Gaussian describing an incident electron beam of width 1.0 eV in energy. The results are shown as the dashed line in Fig. 4. Some gentle undulations survive, particularly in

TABLE I. Positions of calculated resonances (in Ry above the ground state).

^1S	^3S	$^1P^o$	$^3P^o$	^1D	^3D	$^1F^o$	$^3F^o$	^1G	^3G
1.653 82	1.985 70	1.482 81	1.718 34	1.477 02	1.514 73	1.773 65	1.619 07	1.802 10	2.269 73
2.018 62	2.223 38	1.879 56	2.062 46	1.665 96	2.092 47	2.156 95	2.142 98	2.315 83	2.322 53
2.128 25	2.298 75	2.050 30	2.159 37	1.875 16	2.205 00	2.241 76	2.265 98	2.370 29	2.398 92
2.286 83	2.384 40	2.189 98	2.290 82	2.101 12	2.253 54	2.346 56	2.300 80	2.421 04	2.498 57
2.317 87	2.449 12	2.258 98	2.340 27	2.205 76	2.312 38	2.387 14	2.365 22	2.500 42	2.523 38
2.454 62	2.500 22	2.327 27	2.460 45	2.298 32	2.346 02	2.408 82	2.372 65	2.539 54	2.559 71
2.464 66	2.553 99	2.396 28	2.469 61	2.348 85	2.367 18	2.492 60	2.491 05	2.568 76	2.570 96
2.531 33	2.590 92	2.455 19	2.528 48	2.374 72	2.472 55	2.558 83	2.513 12	2.586 48	
2.545 34		2.462 07	2.541 51	2.402 99	2.491 58	2.560 97	2.549 27		
2.592 67		2.483 20	2.552 03	2.480 36	2.540 14	2.576 81	2.556 06		
		2.520 71	2.562 20	2.491 81	2.552 82	2.594 76	2.562 98		
		2.541 71	2.598 20	2.537 68	2.567 42		2.576 62		
		2.548 29		2.589 99					
		2.582 97							

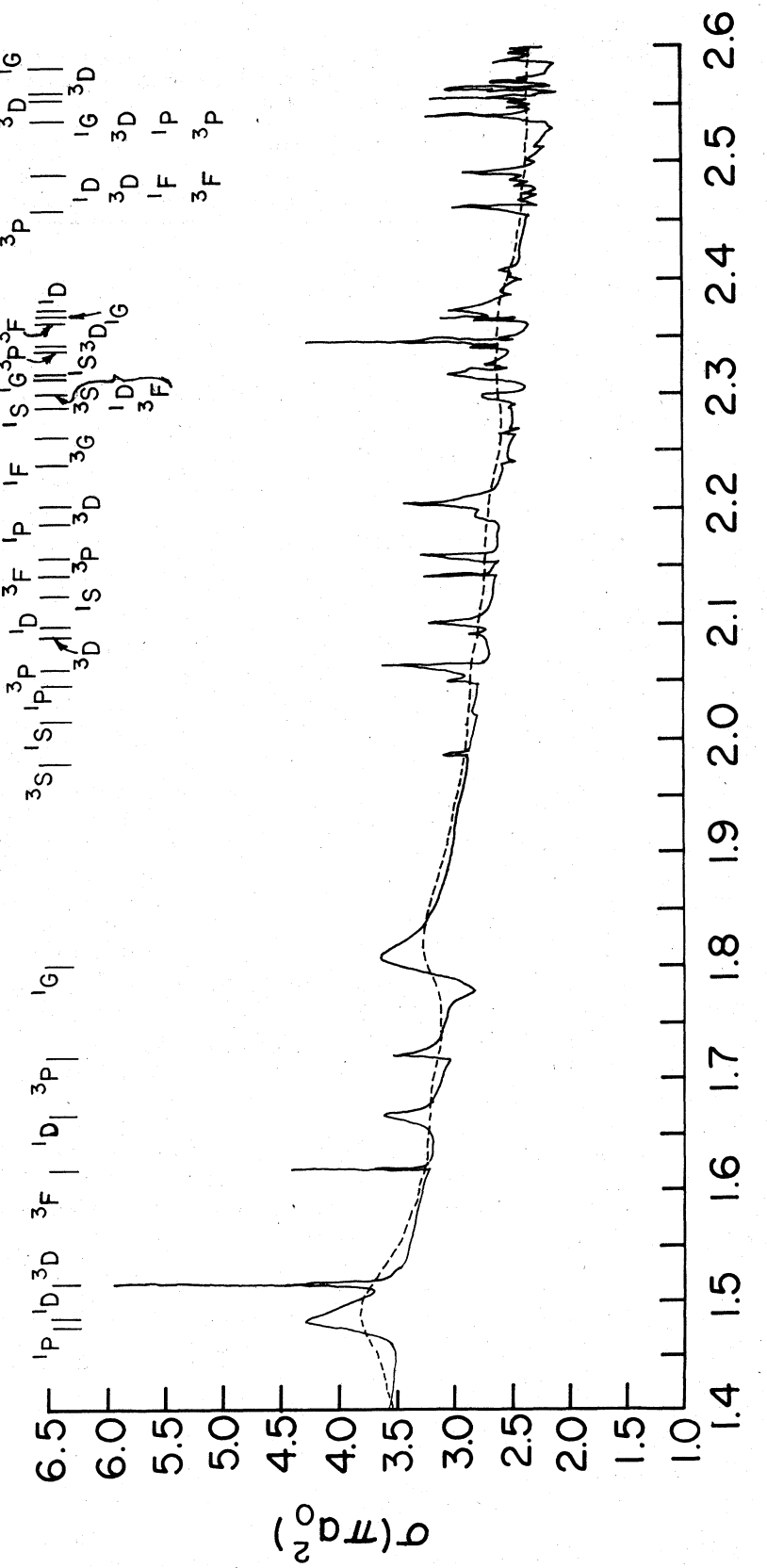

FIG. 4. Total cross section for the $2s$–$2p$ excitation of C^{3+} is shown in units of πa_0^2 as a function of energy of the incident electron from 1.4 to 2.6 Ry (solid line The dashed curve gives the cross section averaged with a Gaussian of width 1 eV to indicate the smearing effect of a distribution of electron energies in the incident beam. Vertical bars indicate the position of major resonances.

TABLE II. Widths (Γ, in Ry) of some of the lower resonances.

Series	E_R	Γ	Series	E_R	Γ
^1S (1)	1.654	0.039	^3S (1)	1.986	0.002
^1S (2)	2.019	0.009	$^3P^o$ (1)	1.718	0.003
$^1P^o$ (1)	1.483	0.023	$^3P^o$ (2)	2.062	0.003
$^1P^o$ (2)	1.880	0.007	^3D (1)	1.515	0.001
$^1P^o$ (3)	2.050	0.001	^3D (2)	2.092	0.001
$^1P^o$ (4)	2.190	0.009	^3D (3)	2.205	0.001
^1D (1)	1.477	0.018	$^3F^o$ (1)	1.619	0.0002
^1D (2)	1.666	0.009			
^1D (3)	1.875	0.009	^3G (1)	2.270	0.0003
^1D (4)	2.101	0.003			
$^1F^o$ (1)	1.774	0.012			
$^1F^o$ (2)	2.157	0.001			
^1G (1)	1.802	0.030			
^1G (2)	2.316	0.007			
^1G (3)	2.370	0.010			

TABLE III. Partial-wave contribution to the $2s \rightarrow 2p$ cross section averaged over the entire range studied (1.4–2.6 Ry). Units are πa_o^2. No resonances have been included for $L \geq 5$.

State	σ (with resonances)	σ (no resonances)
^1S	0.0408	0.0433
^3S	0.0580	0.0580
^1P	0.0995	0.0882
^3P	0.0889	0.0776
^1D	0.0411	0.0078
^3D	0.0129	0.0035
^1F	0.1859	0.1855
^3F	0.1192	0.1137
^1G	0.1517	0.1362
^3G	0.3478	0.3479
$L \geq 5$	(1.764)	1.764
Total	2.910	2.826

the vicinity of the lowest resonances. Hence it may be possible to observe at least some structure in the excitation cross section. However, if the beam width is much greater than 1 eV, all the structure will be washed out.

Finally, we return to the question which prompted this investigation: How important are the resonances? It is evident that if one can observe the excitation process with high resolution, a substantial enhancement can be found. For example, at the peak of the lowest ^3D resonance near 1.5 Ry, the cross section is about 70% above background. However, the resonances are narrow, and in plasmas, one will encounter rather broad energy distribution of electrons. Hence we are led to the following rough estimate. We average the calculated cross section (unweighted) over the energy range from 1.4 to 2.6 Ry. The result is $\sigma_{\text{avg}} = 2.910(\pi a_o^2)$. Then we set all the coefficients $C^{(\lambda)}$ in (3) equal to zero and repeat the process. This cancels all resonances. The result is $\sigma_{\text{avg}}^{(0)} = 2.826(\pi a_o^2)$. Hence the inclusion of resonances can be said to produce a 3% enhancement in the cross section over the range of energies studied. This is a modest effect indeed. It is interesting to see how the various partial waves contribute to these numbers. The breakdown appears in Table III. We see that resonances lead to a large enhancement in the D waves, but these cross sections are small. A small or essentially zero effect is obtained for some waves (^3S, $^1F^o$, ^3G). A negative resonant contribution is found for ^1S.

Results from a two-state close-coupling calculation have previously been reported at two of the energies considered here, 1.4 and 2.2 Ry.[8] At 1.4 Ry, the two-state calculation gives $\sigma = 3.75\pi a_o^2$ for the $2s \rightarrow 2p$ transition while our present result is $\sigma = 3.56\pi a_o^2$. At 2.2 Ry, the two-state result is $2.66\pi a_o^2$. We find pronounced resonances near 2.2 Ry, but a graphical estimate of the nonresonant background at this point gives $\sigma = 2.56\pi a_o^2$. The Gaussian average mentioned previously yields $\sigma = 2.66\pi a_o^2$. It appears that, apart from resonances, the present cross sections are slightly below (4–5%) the two-state values. Evidently, the two-state calculation yields cross sections which are sufficiently accurate for the purpose of calculating reaction rates required in plasma applications.

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