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PHYSICAL REVIEW A

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Electron-Impact Excitation Cross Sections for Atomic Oxygen: $^3P\text{-}3s\ ^3S^0$ *

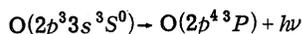
Steven P. Rountree and Ronald J. W. Henry

Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803

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Electron-impact excitation cross sections for $\text{O}(\ ^3P\text{-}3s\ ^3S^0)$ are calculated in unitarized Born, nonexchange, and close-coupling approximations. The close-coupling cross sections have the same energy dependence as measurements by Stone and Zipf but are lower in magnitude by a factor of 4. Two autodetaching levels of $\text{O}^-[2p^3(^4S^0)3s3p\ ^2,^4P]$ are found at 9.67 and 9.94 eV. The doublet state is tentatively identified as a state found experimentally by Edwards at 9.52 eV.

The electron-impact excitation cross section for $\text{O}(\ ^3P\text{-}3s\ ^3S^0)$ is of interest in the atmospheric physics of Earth¹ and Mars.² Fast photoelectrons, produced in the upper atmosphere of the Earth by the absorption of solar ultraviolet radiation by the neutral constituents, lose energy in collision processes. The excitation of the neutral particles produces a substantial component of the dayglow luminosity of the upper atmosphere and the resonance triplet of atomic oxygen



is one of the prominent features.

Recently, an experimental determination of this excitation cross section has been made by Stone and Zipf.³ The only previous theoretical calculation⁴ for this process is based on an impact-parameter method. Stauffer and McDowell's results probably give only an order-of-magnitude estimate in the low-energy region. They predict a broad maximum at 50 eV, which contrasts with Stone and Zipf's measurements of a broad maximum at 20 eV. At high energies, this impact-parameter method gives cross sections of about a factor of 3 higher than experiment. Since these measurements include cascade effects as well as the direct excitation process, they represent an upper limit to the cross section.

We calculate the excitation cross section in the unitarized Born, the nonexchange, and two-state close-coupling approximations. The general

theory of the close-coupling approximation for complex atoms has been given by Smith and Morgan.⁵

We expand the total wave function for the system in a two-state close-coupling expansion in terms of the ground $1s^22s^22p^4(^3P)$ state and the excited $1s^22s^22p^3(^4S)3s(^3S^0)$ state of the oxygen atom. A partial-wave expansion is made for the wave function for the incident electron. The resulting close-coupling equations for the radial motion of the incident electron are solved numerically by using the procedures outlined by Smith, Henry, and Burke.⁶

Since we are considering an optically allowed excitation process, many partial waves contribute to the total inelastic cross section. For large values of the orbital angular momentum of the electron, we calculate the partial cross section in the unitarized Born approximation.⁷ This is a valid procedure since, in the important interaction region, the centrifugal barrier term dominates the direct- and exchange-interaction potentials, and solutions of the radial equations are just spherical Bessel functions.

In the collision problem, the wave functions of the target system are assumed to be known. Kelly⁸ has presented self-consistent-field (SCF) functions in analytical form for oxygen in the configuration $1s^22s^22p^3(^4S^0)3s\ ^3S^0$. Kelly's 3s orbital will be referred to by JsK. An alternative representation of the 3s orbital has been generated

TABLE I. Parameters for the 3s orbital obtained in the frozen-core approximation.

i	C_i	α_i
1	1.124 01	0.449 01
2	-6.732 28	2.609 57
3	-1.437 92	1.458 05

by Hibbert⁹ in the frozen-core approximation. The $1s^2 2s^2 2p^3 (^4S^0)$ core is represented by the oxygen-ion wave functions of Clementi,¹⁰ the exponents in the expansion

$$P_{3s}(r) = \sum_{i=1}^3 C_i r^i e^{-\alpha_i r} \quad (1)$$

are variationally determined, and the coefficients C_i are obtained from the orthonormality conditions. This orbital will be referred to by 3sH and the parameters describing it are given in Table I.

Figure 1 gives the reduced 3s orbital for oxygen versus radial distance. Curves K and H represent the orbitals obtained by Kelly⁸ and Hibbert,⁹ respectively. Curve P gives a function generated by Percival¹¹ in an approximation in which exchange of electrons is neglected. This function was used by Stauffer and McDowell⁴ in their calculation of $O_I(^3P-3s^3S^0)$ cross sections. Since exchange is neglected, the spatial extent of the orbital is too large and hence cross sections calculated with this function will be overestimated.

Unitarized-Born-approximation calculations are made using two independent computer programs. We checked our own program by modifying the program supplied by Hibbert⁹ and using it to calculate the direct interaction potential and hence unitarized-Born-approximation cross sections. Identical results are obtained with these programs.

In addition, the matrix elements that occur in the exchange interaction potential were checked by modifying Hibbert's program.

The sensitivity of the $O_I(^3P-3s^3S^0)$ cross section to the representation of the 3s orbital is investigated in the unitarized Born approximation. Figure 2 presents the cross section as a function of energy for incident electron energies up to 70 eV. Curves K and H represent calculations using 3sK and 3sH functions, respectively. The results agree to within 10%. Since we have the facilities to extend this method to other excited states, the orbitals of which are not currently available in the literature, we have chosen to use the 3sH orbital. For curve N, electron-exchange terms are neglected. The excitation energy has been taken to be the experimental value¹² of 9.52 eV.

The unitarized-Born-approximation cross section increases slowly from threshold and has a broad peak at incident electron energies of 25–40 eV. The nonexchange results peak at a lower energy and more closely follow the energy dependence of the close-coupling calculations except at low energies. Partial cross sections calculated in the nonexchange approximation are within 10% of those obtained in the close-coupling approximation for $l > 3$ and 5, respectively, for incident energies of 1 and 2 Ry. At the highest energies, where all approximations are in good agreement, 40 partial waves are included in order to ensure convergence of the partial-wave expansion.

Near the threshold, the close-coupling results are dominated by a shape resonance which occurs for the 2P and 4P partial waves. An open-channel resonance can occur when centrifugal-barrier, direct, and exchange-interaction potential effects combine to trap temporarily the incident electron in a quasibound state of the system. An analysis

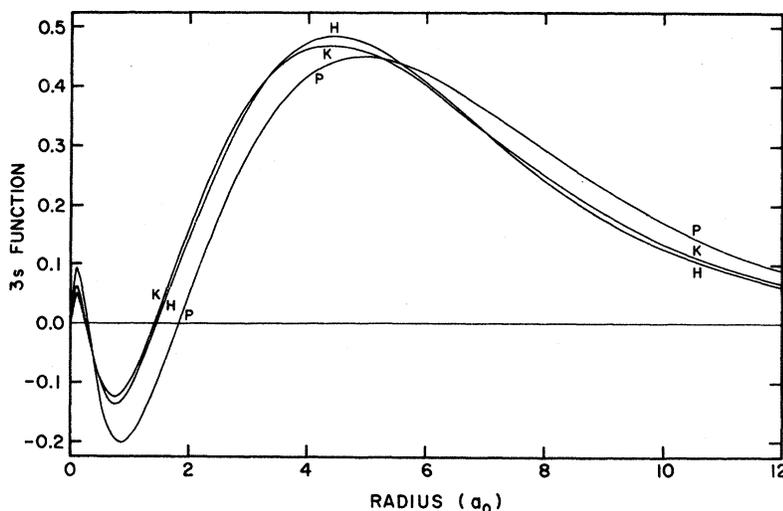


FIG. 1. Oxygen 3s orbitals versus radial distance. Curves K, Kelly (Ref. 8); H, Hibbert (Ref. 9); P, Percival (Ref. 11).

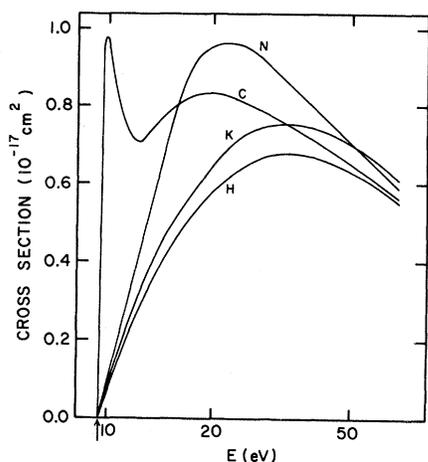


FIG. 2. O I (${}^3P-3s\ 3S^0$) cross section vs energy. Curves K, unitarized Born approximation with $3sK$ orbital; H, unitarized Born approximation with $3sH$ orbital; N, nonexchange approximation; C, close-coupling approximation.

of the partial cross sections indicates that the feature is due to the trapping of outgoing p waves:

$$e^-(l=0) + O({}^3P) \rightarrow O^* [2p^3({}^4S^0)3s({}^3S^0)3p({}^2, {}^4P)] \\ \rightarrow e^-(l=1) + O(3s^3S^0).$$

The approximate resonance positions are 9.67 and 9.94 eV, respectively, for the 2P and 4P channels. These positions will probably shift when additional states are added in the close-coupling expansion. The effect of the neglected states is that of an attractive potential and it is anticipated that the resonance positions will be shifted to lower energies if these states are included.¹³

Two autodetaching states of O^- have been found by Edwards, Risley, and Geballe¹⁴ by observing the electron-energy spectrum of O^- ions excited in collisions with a He target at keV beam energies. The energies of the states have been measured as 10.112 and 12.115 eV. In addition, Edwards¹⁵ has observed further peaks at 9.52 and 13.69 eV. The peak at 9.52 eV may be associated with a $2p^3({}^4S^0)3s3p({}^2P)$ configuration. If the shape resonance which occurs at 9.67 eV were shifted to lower energies, its width would also decrease substantially.

Figure 3 presents the ${}^3P-3s\ 3S^0$ cross section as a function of energy for energies less than 300 eV. Experimental results of Stone and Zipf³ are given by circles. Their measurements are normalized by comparing the optical signal for the atomic excitation with the signal for pure dissociative excitation of O_2 . Absolute cross sections for dissociative excitation by Mumma and Zipf¹⁶ and Lawrence¹⁷ were used as standards. The energy resolution of

Stone and Zipf's experiment is ± 1 eV. The solid curve in Fig. 3 represents a 2-eV average of the close-coupling results given in Fig. 2.

For energies $E > 100$ eV, the cross section exhibits the anticipated behavior of an optically allowed excitation process. It can be well represented by

$$Q({}^3P-3s\ 3S^0) = 0.18 [(\ln k^2)/k^2] (\pi a_0^2),$$

where k^2 is the energy in Ry. The theoretical and experimental cross sections have a similar energy dependence, but the close-coupling results are approximately a factor of 4 smaller than the measurements. Part of the discrepancy is due to cascade contributions, which are included in the measurements. The experiment measures the population of the excited $3s\ 3S^0$ level by all mechanisms, whereas the theoretical results assume that only direct excitation of the ground state by electron impact populates the excited state. A cascade contribution of 30% at 70 eV is estimated¹⁸ in the unitarized Born approximation. At this energy the excitation cross sections calculated in the two-state close-coupling and the unitarized Born approximations agree to within 3% for the same set of orbital functions.

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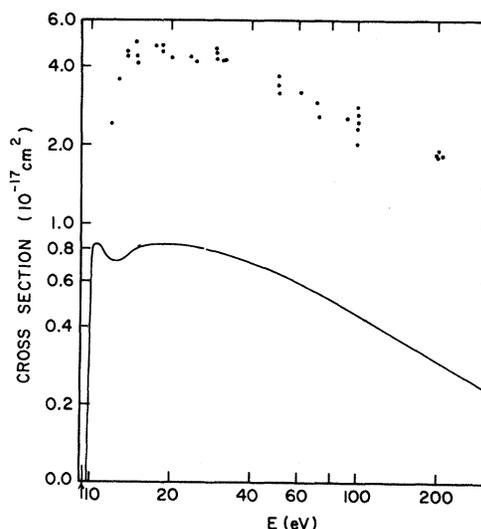


FIG. 3. O I (${}^3P-3s\ 3S^0$) cross section versus energy. Solid curve, close-coupling approximation; circles, measurements of Stone and Zipf (Ref. 3).

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Electron Momentum-Transfer Cross Section in Cesium

William L. Nighan*

United Aircraft Research Laboratories, East Hartford, Connecticut 06108

and

A. J. Postma[†]

Association Euratom-FOM, FOM Instituut voor Plasma-Fysica, Rijnhuizen, Jutphaas, Nederland

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An analysis of electron drift-velocity data in cesium has been conducted in order to determine the electron momentum-transfer cross section. Numerical evaluation of the drift-velocity integral using numerous trial functions for the cross section has revealed the qualitative and semiquantitative nature of the electron momentum-transfer cross section in cesium. The cesium cross section found to be most consistent with the available experimental data exhibits considerable variation with electron energy in the range 0.1–1.0 eV, the region of primary importance in plasma applications.

I. INTRODUCTION

The Frost-Phelps technique^{1,2} for the determination of low-energy electron cross sections from analysis of transport coefficients is well known.^{3,4} With this method, electron momentum-transfer cross sections have been obtained for most of the noble gases² and the more common atmospheric gases^{5,6} in the electron energy range 0.01–10.0 eV, the region of primary importance in plasma problems. The principal requirement for successful application of the method is the availability of accurate electron transport data over a broad range of average electron energy. Fortunately, the available data for many species of interest^{2,5,6} possess an absolute accuracy on the order of ± 5 –10% over a several-order-of-magnitude variation of the parameter E/N ,⁷ thereby permitting

determination of the momentum-transfer cross section to an accuracy of approximately 15–30% over a wide range of electron energy. In fact, Crompton *et al.*⁸ have obtained the momentum-transfer cross section for electrons in He in the 0.01–3.0-eV range to an accuracy of ± 2 % utilizing drift-velocity data accurate⁹ to ± 1 %. This work also contains an excellent description of the experimental and analytical uncertainties associated with the procedure, which by this time has become established as the most effective method of electron cross-section determination in the very-low-energy regime.

During the past several years, electron drift-velocity data have become available^{10–12} for cesium. However, the available data exist over a limited range of energy and possess an absolute accuracy which is in the 25–50% range at best; a condition