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Electron impact excitation cross sections for phosphorus

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Abstract. An analytic atomic independent-particle-model is used to generate wave functions for the valence and excited states of the neutral phosphorus atom. These wave functions are used to calculate generalized oscillator strengths, and from these quantities the cross sections are obtained in Born approximation. Various excitations from the $3p^3(^4S_{3/2})$ ground state are considered, and results are presented for electron impact energies up to 5 keV.

PACS. 34.10.+x General theories and models of atomic and molecular collisions and interactions (including statistical theories, transitions state, stochastic and trajectory models, etc. – 34.80.Dp Atomic excitation and ionization by electron impact

1 Introduction

Neutral phosphorus is of astrophysical interest [1], as well as being of interest in laser devices [2]. Therefore a complete and accurate knowedge of its atomic properties is essential. Atomic cross sections are needed as input data for problems in applied atomic physics such as electron energy deposition in a gas. In such problems the totality of all elastic and inelastic cross sections is needed, *e.g.* excitation, ionization, dissociation, dissociative excitation, multiple ionization, *etc.* Very little experimental information is available on atomic cross sections, consequently theory must be relied on for the most part. In this work we calculate excitation cross sections for electron collisions with phosphorus atoms. These cross sections may be useful as partial input data for the type of application mentioned above. We first obtain the generalized oscillator strengths and then use these quantities to obtain the cross sections. Excitations from the ground state $3p^3(^4S_{3/2})$ to various s, p, d excited states are considered.

The method of calculation is described below.

2 Method of calculation

The phosphorus atom is a 15-electron system which may be treated by an independent-particle-model approach. In this model each electron moves independently in an effective potential having the form

$$V(r) = -(2/r)\{14[H(\mathrm{e}^{r/d} - 1) + 1]^{-1} + 1\} \qquad (1)$$

where r is the electron-nucleus distance in units of the Bohr radius, $V(r)$ is in Rydbergs, and d, H are adjustable parameters.

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This potential is substituted into the radial Schrödinger equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} - V(r) + E_{nl}\right) P_{nl}(r) = 0 \qquad (2)$$

which is then solved to obtain the energy eigenvalues E_{nl} and wave funtions $P_{nl}(r)/r$. The parameters d, H are determined by fitting the eigenvalues to the experimental single-particle energy levels. The values $d = 1.4088$ and $H = 4.7988$ were obtained for the best fit.

3 Generalized oscillator strengths

The cross sections are obtained from the Generalized Oscillator Strengths (GOS). The general formula for the GOS is

$$f(x) = N_0 F^2 \sum_L (2l+1)(2L+1) \begin{pmatrix} l_0 & l & L \\ 0 & 0 & 0 \end{pmatrix}^2 S_L^2 \qquad (3)$$

where

$$S_L = \xi^{-1/2} \int_0^\infty P_{n_0 l_0}(r) j_L(Kr) P_{nl}(r) \mathrm{d}r. \qquad (4)$$

The dimensionless quantity x is the square of the momentum transferred between the initial state $n_0 l_0$ and the final state nl : $x = K^2 a_0^2$ (a_0 is the Bohr radius). The quantity ξ is the reduced square of momentum transfer: $\xi = x/x_\mathrm{t}$; here x_t is the transition energy. The quantity N_0 is the number of valence electrons, and F is the coefficient of fractional parentage for constructing the initial state from the core state and an $n_0 l_0$ electron. The array in large

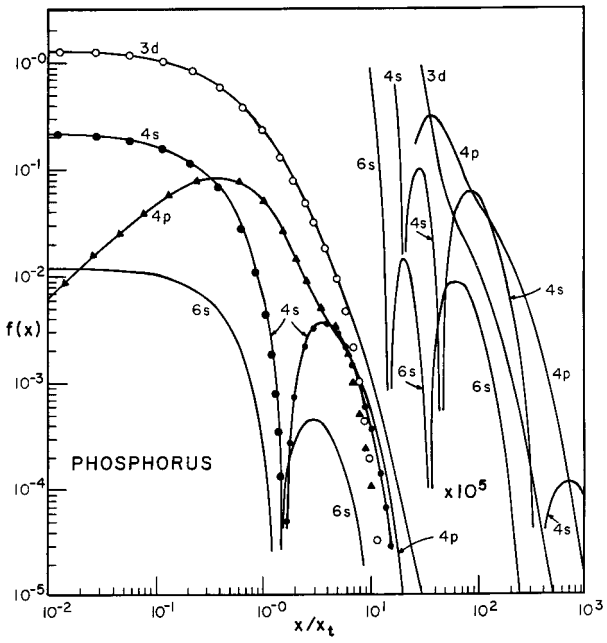

Fig. 1. GOS for 3p-ns, 3p-np and 3p-nd transitions in P as functions of reduced square of momentum transfer. The curves are the results of the present calculations. The solid dots (•), open circles (o), and triangles (▲) are representative fits using equations (5 and 6). Values of the GOS below 10^{-5} have been multiplied by 10^5.

brackets in equation (3) is a $3j$ symbol and $j_L(Kr)$ in equation (4) is a spherical Bessel function.

Plots of the GOS are shown in Figure 1. As ξ increases, the GOS for the transitions 3p-ns decrease in an oscillatory manner, while the GOS for 3p-nd decrease monotonically. The GOS for 3p-np also decrease monotonically but pass through a maximum first.

The calculation of cross sections can be facilitated by parametrizing the GOS with simple analytic forms:

$$f(\xi) = A(\mathrm{e}^{-\alpha\xi} + \beta\xi\mathrm{e}^{-\gamma\xi})^2 \text{ for 3p}-\text{ns, 3p}-\text{nd}, \quad (5)$$

$$f(\xi) = \xi A(\mathrm{e}^{-\alpha\xi} + \beta\xi\mathrm{e}^{-\gamma\xi})^2 \text{ for 3p}-\text{np}. \quad (6)$$

Here the quantities A, α, β, γ are adjustable parameters which are varied to obtain the best fit to the numerical GOS. The quantity A in equation (5) is the optical oscillator strength, which is the limit of the GOS as $\xi \to 0$. When using equation (5), A is assigned the value of the optical oscillator strength and three-parameter fits are obtained. Four-parameter fits are obtained when using equation (6). The values of the four parameters which yield the best fits are given in Table 1. Sample fits are shown in Figure 1. Equations (5 and 6) actually only reproduce the GOS where it is significantly large ($f(x) > 10^{-5}$).

Table 1. Values of the dimensionless parameters A, α, β, γ in equations (5 and 6).

3p to	A	α	β	γ
4s	0.2245	1.3034	−0.1318	0.3460
5s	0.0337	0.7527	−0.4874	0.5750
6s	0.0121	0.7388	−0.4720	0.5758
4p	0.5884	0.5289	−0.7322	0.9098
3d	1.3508	1.2978	0.2283	0.5263
4d	0.3381	0.9215	0.1076	0.3611
5d	0.1331	0.7966	0.0729	0.3016

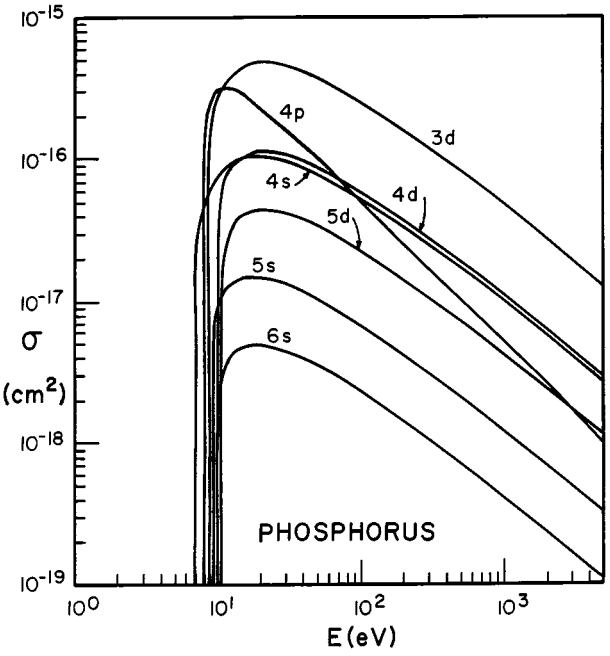

Fig. 2. Integrated cross sections for 3p-ns, 3p-np, 3p-nd excitations in P *vs.* electron impact energy.

4 Cross sections

In Born approximation, the integrated cross section is obtained from the GOS using the formula

$$\sigma = \frac{q_0}{WE}\int_{\xi_l}^{\xi_u}\frac{f(\xi)}{\xi}\mathrm{d}\xi \quad (7)$$

where W, E are the excitation energy and incident electron energy in eV, respectively, and

$$q_0 = 6.514 \times 10^{-14}\ \mathrm{cm}^2\ \mathrm{eV}^2,$$

and

$$\xi_{u,l} = (2E/W)[1 \pm (1 - W/E)^{1/2} - W/2E]. \quad (8)$$

Now equations (5 and 6) correspond, respectively, to the first three and the first four terms of the expansion

$$f(\xi) = \sum_{s=0}^{\infty} f_s \xi^s \exp(-\alpha_s \xi). \quad (9)$$

Table 2. Comparison between oscillator strengths from the present calculations and those from experiment and other calculations for the transitions $3p^3(^4S_{3/2}) \longrightarrow 3p^2(^3P)\ ns\ (^4P)$ for $n \leq 4 \leq 7$, and $3p^3(^4S_{3/2}) \longrightarrow 3p^2(^3P)\ nd\ (^4P)$ for $3 \leq n \leq 7$, in PI.

3p to	Present Calculations	Other Calculations	Experiment
4s	0.2245	0.20[d]	0.30 ± 0.03[a]
		0.256[e]	0.31 ± 0.04[b]
		0.318[f]	0.36 ± 0.03[c]
		0.4545[g]	
5s	0.0337	0.049[f]	
6s	0.0121	0.041[f]	
7s	0.0058		
3d	1.3508	0.066[f]	
		0.9998[g]	
4d	0.3381	0.216[f]	
5d	0.1331	0.122[f]	
6d	0.0664	0.075[f]	
7d	0.0382		

[a][4]; [b][5]; [c][6]; [d][7]; [e][8]; [f][9]; [g][1].

On substituting equation (9) into equation (7), a closed-form expression involving standard mathematical functions is obtained for the cross section:

$$\sigma(E) = \frac{q_0}{WE}\big(f_0[E_1(\alpha_0\xi_l) - E_1(\alpha_0\xi_u)] + \sum_{s=1}^{\infty}\frac{f_s}{\alpha_s^s}[\gamma(s,\alpha_s\xi_u) - \gamma(s,\alpha_s\xi_l)]\big). \quad (10)$$

In equation (10), E_1 is the first exponential integral function, and $\gamma(s,y)$ is the incomplete *gamma* function. The first term is dominant at high energies and leads to the $E^{-1}\ln E$ dependence associated with the Born approximation.

The cross sections are presented in Figure 2. Direct comparison with experiment is not possible due to lack of experimental data. However, we can estimate the accuracy of our results by looking at the accuracy of the oscillator strengths. The Born cross sections are very sensitive to the values of the oscillator strengths [3]. In Table 2 we present a comparison between the oscillator strengths from the present calculations and those obtained from experiment and other calculations. Three experimental values are available for the 3p-4s transition: 0.30 ± 0.03 from the work of Curtis *et al.* [4], 0.31 ± 0.04 from the work of Savage and Lawrence [5] and 0.36 ± 0.03 from the work of Livingston *et al.* [6]. The value obtained from the present calculations, 0.2245, is within 17% to 42% of these experimental values. There are no experimental data for the other transitions. Also included in Table 2 are some values from other calculations. For the 3p-4s transition, our value 0.2245 compares favorably with the values 0.20 obtained by Gruzdev and Prokofev [7] using the Coulomb appoximation, 0.256 obtained by Ho and Henry [8] using Hartree-Fock wave functions, 0.318 obtained by Mukherjee and Ohno [9] using time-dependent coupled Hartree-Fock theory, and 0.4545 obtained by Fawcett [1] using a Hartree-Fock - Relativistic program. For the higher transitions our values are comparable to those obtained in other calculations except in the case 3p-3d where the discrepancies among the theoretical results are more substantial. Based on the direct comparison with experiment for 3p-4s transition, we can say that our high-energy cross sections have an estimated accuracy of between 17% and 42%, but our low-energy cross sections are expected to be inaccurate due to the fact that the Born approximation is poor near the threshold of inelastic scattering.

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