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Photoionization of ground and excited levels of P II

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HIGHLIGHTS

- Presents detailed study with resonant features of photoionization of P II.
- Found prominent resonant structures and enhancement in background.
- Relativistic effect introduced important resonance at ionization threshold.
- Study considers for many excited energy levels with $n<10$ for complete modeling.
- Relativistice Breit–Pauli R-matrix method has yielded high precision atomic data.

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ABSTRACT

Photoionization cross section (σ_{PI}) of P II, ($h\nu$ + P II → P III + e), from ground and a large number of excited levels are presented. The study includes the resonant structures and the characteristics of the background in photoionization cross sections. The present calculations were carried out in the Breit–Pauli R-matrix (BPRM) method that includes relativistic effects. The autoionizing resonances are delineated with a fine energy mesh to observe the fine structure effects. A singular resonance, formed by the coupling of channels in fine structure but not allowed in LS coupling, is seen at the ionization threshold of photoionization for the ground and many excited levels. The background cross section is seen enhanced compared to smooth decay for the excited levels. Examples are presented to illustrate the enhanced background cross sections at the energies of the core levels, $^4P_{3/2}$ and $^2D_{3/2}$, that are allowed for electric dipole transitions by the core ground level $^2P^o_{1/2}$. In addition strong Seaton or photo-excitation-of-core (PEC) resonances are found in the photoionization of single valence electron excited levels. Calculations used a close coupling wave function expansion that included 18 fine structure levels of core P III from configurations $3s^23p$, $3s3p^2$, $3s^23d$, $3s^24s$, $3s^24p$ and $3p^3$. Photoionization cross sections are presented for all 475 fine structure levels of P II found with $n \leq 10$ and $l \leq 9$. The present results will provide high precision parameters of various applications involving this less studied ion.

1. Introduction

Phosphorus is part of our daily life in variety of applications. Being an element of RNA where it plays a role in signal passing, it is also a basic element like carbon, oxygen in the evolution of life. However, its astrophysical abundance is low and is difficult to detect due to lack of data. Its existence in astronomical objects has been found in damp Galaxies by Molaro et al. (2001) and by Welsh et al. (2001). Compared to other elements, only very limited theoretical study has been carried out on the radiative processes of this element.

Photoionization cross sections of Si-like ions, isoelectronic to P II, have been reported under the (OP, 1996) by Mendoza and Zeippen (1988); Nahar and Pradhan (1993). However, P which is the next element to Si in the periodic table, was not studied due to lower abundance in astrophysical plasmas. Photoionzation cross section of P II has been measured recently with high precision at the Advanced Light Source (ALS) by Hinojosa et al. (2015) where they studied the low energy features in detail. The observed features were identified theoretically using R-matrix method and were found to be produced by low lying fine structure levels that belong to ground configuration $3s^23p^2$ and one metastable state $3s3p^3(^5S^o_2)$. The present work reports full scale study of features of photoionization, such as, background enhancement, photo-excitation-of core resonances, and reporting cross sections of a large number of excited levels, 475 in total with n ≤ 10 as needed for spectral modelings. In contrast to the study of photoionization

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of Si-like ions in non-relativistic LS coupling (Nahar and Pradhan, 1993), the present study employed the Breit-Pauli R-matrix (BPRM) method with relativistic effects developed under the Iron Project Hummer et al. and includes radiation damping effect of resonances (Zhang et al., 1999).

2. Theory

Photoionization process can be direct as,

$$h\nu + X^+ \rightarrow e + X^{2+}. \quad (1)$$

However, depending on the photon energy which matches the energy of a state belonging to Rydberg series of states below an excited core state but lying above the ionization threshold, an intermediate doubly excited autoionizing state can form before ionization,

$$h\nu + X^+ \leftrightharpoons (X^+)^{**} \leftrightharpoons e + X^{2+} \quad (2)$$

Formation of an autoionizing state can lead to a resonance in photoionization and is the main cause for introduction of features and structures in the process.

Theoretically the resonances can be generated naturally in an ab initio manner by including the core excitations in the wave function, as considered in the close coupling (CC) approximation. In CC approximation, the atomic system is represented by a (N+1) number of electrons where the core ion is an N-electrons system interacting with the (N+1)th electron. The (N+1)th electron can be bound or in the continuum depending on its negative or positive energy (E). The total wave function, Ψ_E, in a symmetry $SL\pi$ of the system is expressed by an expansion as (e.g. Pradhan and Nahar, 2011)

$$\Psi_E(e + ion) = A \sum_i \chi_i(ion)\theta_i + \sum_j c_j \Phi_j, \quad (3)$$

where χ_i is the core ion eigenfunction representing ground and various excited states and the sum is over the number of core states considered. The core is coupled with the (N+1)th electron function, θ_i. The (N+1)th electron with kinetic energy k_i^2 is in a channel labeled as $S_iL_i(J_i)\pi_i k_i^2 \ell_i[SL(J)\pi]$. A is the antisymmetrization operator. In the second sum, the Φ_js are bound channel functions of the (N+1)-electrons system that provides the orthogonality between the continuum and the bound electron orbitals and account for short range correlation. Substitution of $\Psi_E(e + ion)$ in the Schrodinger equation

$$H_{N+1}^{BP}\Psi_E = E\Psi_E \quad (4)$$

introduces a set of coupled equations that are solved using the R-matrix approach. The details of the R-matrix method in the CC approximation can be found in, e.g. (Burke and Robb, 1975; Seaton, 1987; Berrington et al., 1987; 1995; Pradhan and Nahar, 2011). The relativistic effects are included through Breit-Pauli approximation (e.g. Pradhan and Nahar, 2011) where the Hamiltonian is given by

$$H_{N+1}^{\rm BP} = \sum_{i=1}^{N+1}\left\{-\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N+1}\frac{2}{r_{ij}}\right\} + H_{N+1}^{\rm mass} + H_{N+1}^{\rm Dar} + H_{N+1}^{\rm so}, \quad (5)$$

in Rydberg unit. The relativistic correction terms are mass correction, $H^{\rm mass} = -\frac{\alpha^2}{4}\sum_i p_i^4$, Darwin, $H^{\rm Dar} = \frac{Z\alpha^2}{4}\sum_i \nabla^2(\frac{1}{r_i})$, and spin-orbit interaction, $H^{\rm so} = Z\alpha^2\sum_i \frac{1}{r_i^3}\mathbf{l_i}.\mathbf{s_i}$. R-matrix Breit–Pauli (BPRM) approximation also includes part of two-body interaction terms, such as the ones without the momentum operators (Pradhan and Nahar, 2011). In BPRM method the set of $SL\pi$ is recoupled for $J\pi$ levels of (e + ion) system in intermediate coupling which is followed by diagonalization of the Hamiltonian.

Table 1
Levels and energies (E_t) of core ion P III included in the wave function expansion of P II. Calculated energies from SUPERSTRUCTURE (SS) are compared with those in the compiled table of NIST.

Level		J_t	E_t(Ry) NIST	E_t(Ry) SS
1	$3s^23p(^2P^o)$	1/2	0.0	0.
2	$3s^23p(^2P^o)$	3/2	0.005095	0.00429
3	$3s3p^2(^4P)$	5/2	0.523559	0.51278
4	$3s3p^2(^4P)$	3/2	0.520570	0.51028
5	$3s3p^2(^4P)$	1/2	0.518708	0.50874
6	$3s3p^2(^2D)$	3/2	0.682693	0.70551
7	$3s3p^2(^2D)$	5/2	0.682957	0.70565
8	$3s3p^2(^2S)$	1/2	0.913094	0.99414
9	$3s3p^2(^2P)$	1/2	0.993621	1.03335
10	$3s3p^2(^2P)$	3/2	0.997044	1.03613
11	$3s^23d(^2D)$	3/2	1.065039	1.14381
12	$3s^23d(^2D)$	5/2	1.065142	1.14392
13	$3s^24s(^2S)$	1/2	1.073800	1.10909
14	$3s^24p(^2P^o)$	1/2	1.28832	1.34867
15	$3s^24p(^2P^o)$	3/2	1.28956	1.34955
16	$3p^3(^2D^o)$	3/2	1.342508	1.38637
17	$3p^3(^2D^o)$	5/2	1.343073	1.38678
18	$3p^3(^4S^o)$	3/2	1.455433	1.49071

For an electron with positive energies (E > 0) the solution of the BPRM method is a continuum wave function, Ψ_F and with negative energy (E ≤ 0) it is a bound state, Ψ_B. The complex resonant structures in photoionization are produced from couplings between continuum channels that are open ($k_i^2 > 0$), and bound channels that are closed ($k_i^2 < 0$), at electron energies k_i^2 which correspond to autoionizing states of the Rydberg series, $S_iL_iJ_i\pi_i\nu\ell$. where ν is the effective quantum number of the series converging to excited core thresholds $S_iL_iJ_i\pi_i$.

The photoionization cross section (σ_{PI}) is given by (e.g. Pradhan and Nahar, 2011)

$$\sigma_{PI} = \frac{4\pi^2}{3c}\frac{1}{g_i}\omega\mathbf{S}, \quad (6)$$

where g_i is the statistical weight factor of the bound state, ω is the incident photon energy and $\mathbf{S}$ is the generalized line strength

$$\mathbf{S} = |\langle\Psi_f||\mathbf{D}_L||\Psi_i\rangle|^2 = \left|\left\langle\psi_f\left|\sum_{j=1}^{N+1} r_j\right|\psi_i\right\rangle\right|^2, \quad (7)$$

where Ψ_i and Ψ_f are the initial and final state wave functions, and $\mathbf{D}_L$ is the dipole operator in length form.

3. Computations

BPRM computations are carried out using the R-matrix package of codes (Berrington et al., 1995; Nahar and Pradhan, 1994; Zhang et al., 1999) for various stages. They are initiated with the wave function of the core as the initial input. The core wave function for P III was obtained from atomic structure calculations using code SUPERSTRUCTURE (SS) (Eissner et al., 1974; Nahar et al., 2003). SS uses Thomas–Fermi–Dirac–Amaldi potential and includes relativistic contributions in Breit–Pauli approximation. Table 1 presents ground and 17 excited fine structure levels of P III included in the wave function expansion of P II. They were obtained from optimization of 19 configurations up to 5s orbital of P III, $3s^23p(1)$, $3s3p^2(2)$, $3s^23d(3)$, $3s^24s(4)$, $3s^24p(5)$, $3p^3(6)$, $3s3p3d(7)$, $3s^24d(8)$, $3s^24f(9)$, $3s^25s(10)$, $3s3p4s(11)$, $3s3p4p(12)$, $3s3p4d(13)$, $3s3p4f(14)$, $3p^23d(15)$, $3p^24s(16)$, $3p^24p(17)$, $3p^24d(18)$, $3p^24f(19)$. The calculated energies from SS are compared with observed values (listed