



# ***P*-wave Electron-Be<sup>3+</sup>, C<sup>5+</sup>, and O<sup>7+</sup> Elastic Scattering and Photoabsorption in Two-Electron Systems**

Research Article

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**Abstract.** In previous papers [Bhatia, Phys. Rev. A **85**, 052708 (2012); **86**, 032709 (2012); **87**, 042705 (2013)] electron-hydrogen, electron-He<sup>+</sup>, electron-Li<sup>2+</sup> *P*-wave scattering phase shifts were calculated using the variational polarized orbital theory. This method is now extended to the singlet and triplet *P*-wave scattering from Be<sup>3+</sup>, C<sup>5+</sup> and O<sup>7+</sup> in the elastic region. The long-range correlations are included in the Schrödinger equation by using the method of polarized orbitals **variationally**. Phase shifts are compared to those obtained by other methods. The present calculation provides results which are rigorous lower bounds to the exact phase shifts. Using the presently calculated *P*-wave continuum functions, photoionization of the singlet and triplet *S* states of Be<sup>2+</sup>, C<sup>4+</sup>, and O<sup>6+</sup> are also calculated, along with the radiative recombination rate coefficients at various electron temperatures.

**Keywords.** Electron scattering; Photoionization

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## **1. Introduction and Calculations**

Collision between an electron and a target is a many-body problem. The perturbation in the target due to the incident electron induces in it electric multipole moments. The exact knowledge of the single-electron targets makes it possible to obtain accurate results for various quantities. In general, it is not possible to infer phase shifts, resonance parameters, photoabsorption cross sections, radiative-attachment rates, and cross sections for free-free absorption of radiation by scaling as the nuclear charge increases. This is due to the fact that the attractive Coulomb

interactions and the repulsive electron-electron interactions cannot be scaled the same way with respect to the nuclear charge. Phase shifts are also required in the calculations of laser-assisted free-free transitions in electron-atom collisions [1, 2]. Therefore, it becomes important to carry out calculations in each case.

At low energies, in addition to the exchange between the electrons, the distortion of the target produced by the incident electrons is important. This distortion can be taken into account by the method of polarized orbitals [3, 4] which includes the effect of polarization in the ansatz of the wave function of the target. Other approximations for calculating phase shifts are: Kohn-Feshbach variational method [5], Kohn variational method [6], *R*-matrix method [7], and the finite element method [8]. The electron-hydrogenic systems *P*-wave phase shifts in the elastic region have been calculated by Sloan [9] and by Khan et al. [10] using the method of polarized orbitals and by Gien [11, 12] using the Harris-Nesbet method. The electron-H, electron-He<sup>+</sup>, and electron-Li<sup>2+</sup> *S*-wave and *P*-wave phase shifts in the elastic region have been calculated [13–17] in which the long-range potential proportional to  $-1/r^4$  was included **variationally**.

Photoionization and its reverse process, radiative recombination, in atoms and ions are needed in the solar and in the stellar modeling of the opacity. Photoionization of heavy elements is important in astrophysical modeling because they are more abundant than the lighter elements. This process is also important in the upper atmosphere, and the cross sections are required to model fission and fusion plasmas. Photoionization cross sections of O<sup>6+</sup> are of interest in x-ray spectroscopy of astrophysics and in laboratory. Electron-electron correlations in various systems can be investigated by the process of photoionization of atoms and ions.

Since the excited states have lower threshold energies for ionization, much less photon energy is required for photoionization of these states. The photoelectrons emitted from photoionized states then excite various levels of the plasma constituents which decay to the lower levels, providing spectra of various astrophysical objects for diagnostic purposes. The observations of such spectra help to infer the electron densities, temperatures, and element abundances of the astrophysical plasmas.

It is also possible for the photoionized system to be left in excited states. These states could decay to the lower states emitting photons of various wavelengths. Of particular interest is the absorption of photons in H<sup>-</sup> and He targets which are left in the *2p* state after photodetachment and photoionization. The remaining H atom and He ion emit Lyman-alpha and 304 Angstrom radiation [18]. The Lyman-alpha radiation has been observed recently from the Milky Way galaxy [19]. We use Rydberg units: energy in Rydberg, length in Bohr radius  $a_0$ , and phase shifts in radians.

We briefly describe the formalism already discussed in previous papers on *S* and *P* scattering states. In order to obtain the Schrödinger equation, the total spatial wave function for electron-target partial wave (denoted by *L*) problem is written as

$$\Psi_L(\vec{r}_1, \vec{r}_2) = \frac{u(r_1)}{r_1} Y_{L0}(\hat{r}_1) \Phi^{pol}(r_1, r_2) \pm (1 \leftrightarrow 2). \quad (1.1)$$

The ( $\pm$ ) above refers to singlet (upper sign) or triplet (lower sign) scattering, respectively. The effective target wave function can be written as

$$\Phi^{pol}(\vec{r}_1, \vec{r}_2) = \phi_0(\vec{r}_2) - \frac{\chi_\beta(r_1)}{r_1^2} \frac{u_{1s \rightarrow p}(r_2)}{r_2} \frac{\cos(\theta_{12})}{\sqrt{Z\pi}}, \quad (1.2)$$

where

$$\phi_0(\vec{r}_2) = \sqrt{\frac{Z^3}{\pi}} e^{-Zr_2}, \tag{1.3}$$

$$u_{1s \rightarrow p}(r_2) = e^{-Zr_2} \left( \frac{Z}{2} r_2^3 + r_2^2 \right), \tag{1.4}$$

and  $\theta_{12}$  is the angle between  $\vec{r}_1$  and  $\vec{r}_2$ . We have replaced the step function  $\varepsilon(r_1, r_2)$ , used by Temkin [4], by a smooth cutoff function  $\chi_\beta(r_1)$  which is of the form

$$\chi_\beta(r_1) = (1 - e^{-\beta r_1})^n, \tag{1.5}$$

where  $n \geq 3$ . Now the polarization of the target takes place whether the scattered electron is inside or outside the orbital electron. The polarization function given in Eq. (1.2) is valid throughout the range. This is unlike the step function  $\varepsilon(r_1, r_2)$  used in [4] which ensures that the polarization takes place when the scattered electron  $r_1$  is outside the orbital electron  $r_2$ . Furthermore, the function in Eq. (1.5) gives us another parameter  $\beta$ , which is a function of  $k$ , the incident electron momentum. This term guarantees that  $\chi_\beta(r_1)/r_1^2 \rightarrow 0$  when  $r_1 \rightarrow 0$  and it also contributes to the short-range correlations, and therefore, is useful to optimize the results.

Beyond the terms containing  $u(r)$  explicitly, are the terms giving rise to the exchange approximation, here  $L = 1$ . The scattering function  $u(r)$  is obtained by solving the integrodifferential equations resulting from

$$\int \left[ Y_{10}^*(\Omega_1) \Phi^{pol}(\vec{r}_1, \vec{r}_2) (H - E) \Psi_L \right] d\vec{r}_2 = 0. \tag{1.6}$$

In the above equation  $H$  is the Hamiltonian and  $E$  is the total energy of electron-target scattering system:

$$H = -\nabla_1^2 - \nabla_2^2 - \frac{2Z}{r_1} - \frac{2Z}{r_2} + \frac{2}{r_{12}}, \tag{1.7}$$

$$E = k^2 - Z^2, \tag{1.8}$$

$k^2$  is the kinetic energy of the incident electron and  $Z$  is the nuclear charge. The integrodifferential equations are solved by the noniterative method [20]. The phase shifts are inferred by knowing the scattering function at

$$r \equiv r_1 \rightarrow \infty, \tag{1.9}$$

$$\lim_{r \rightarrow \infty} u(r) \propto \sin \left[ kr + \frac{l(l+1)}{r^2} + \frac{Z-1}{k} \ln(2kr) + \arg \Gamma \left( 1 - \frac{i(Z-1)}{k} \right) + \eta \right].$$

The phase shifts for  $^3P$  and  $^1P$  scattering states for e-hydrogenic beryllium, given in Table I, are compared with those obtained in [10] using the method of polarized orbitals. Khan et al. [10] took into account the exchange-polarization terms in the calculation. The present results for the triplet states are lower than those obtained in [10] for lower values of  $k$ , but higher for the singlet states. The results in [10] have no variational bounds while the present results have

variational lower bounds and therefore are accurate compared to those of [10]. In Table II, phase shifts for e-C<sup>5+</sup> and e-O<sup>7+</sup> are given. The phase shifts for all the three ions are always positive for the triplet states and negative for the singlet states. It has not been possible to calculate accurately phase shifts at  $k = 0.1$  for e-C<sup>5+</sup> and e-O<sup>7+</sup> because the Coulomb field dominates at this energy and integrating the integrodifferential equation too far results into inaccuracies. Therefore, the continuum wave function is not known for further calculations at  $k = 0.1$  for these two ions.

**Table I.** Comparison of phase shift  $\eta$  (radians) for e-Be<sup>3+</sup> scattering with the polarized orbital results [10]

$k$	Be <sup>2+</sup> , <sup>3</sup> P	Pol. Orb [10]	Be <sup>2+</sup> , <sup>1</sup> P	Pol. Orb [10]
0.1	1.2940(-1)		-4.0516(-2)	
0.2	1.2927(-1)		-4.0494(-2)	
0.3	1.2925(-1)		-4.0404(-2)	
0.4	1.2895(-1)	1.2991(-1)	-4.0268(-2)	-4.6460(-2)
0.5	1.2919(-1)	1.2977(-1)	-3.9967(-2)	-4.4800(-2)
0.9	1.2815(-1)		-3.8943(-2)	
1.0	1.2854(-1)	1.2861(-1)	-3.7995(-2)	-3.2800(-2)
1.5	1.2655(-1)	1.2651(-1)	-3.4790(-2)	-1.9360(-2)
1.8	1.2365(-1)	1.2476(-1)	-3.2114(-2)	-1.3480(-2)
2.0	1.2411(-1)	1.2336(-1)	-2.9177(-2)	-1.1180(-2)
2.5	1.2202(-1)	1.1912(-1)	-2.2472(-2)	-1.1270(-2)
2.8	1.1973(-1)	1.1612(-1)	-1.8138(-2)	-1.3040(-2)
3.2	1.1606(-1)	1.1187(-1)	-1.2392(-2)	-8.7900(-2)
3.3	1.5016(-1)		-1.1026(-2)	
3.5	1.1280(-1)		-8.3387(-3)	

## 2. Photoionization of Two-Electron Systems

Photoionization processes are important in the study of the upper atmosphere physics and for stellar modeling. The dominant processes determining the ionization structure of any plasma are photoionization (in addition to collisional ionization) and its inverse process, radiative recombination. These two processes are important to investigate the ionization balance in a plasma. In a previous paper [17], we calculated the photoabsorption cross sections of  $S$ -states of two-electron systems: H<sup>-</sup>, He and Li<sup>+</sup>. In this process, the final continuum state of the photoelectron is the  $P$ -state when the target is left in the ion-ground state. It is known that the opacity in the sun is due to the photodetachment of H<sup>-</sup>. The general expression for the cross section at low photon energies (below 1000 eV) is given, in the dipole approximation, by

$$\sigma(l_f) = \frac{4\pi(2l_f + 1)\alpha k\omega}{3(2l_i + 1)} |\langle \Psi_{l_f} | z_1 + z_2 | \Phi_i \rangle|^2, \quad (2.1)$$

where  $\alpha$  is the fine-structure constant,  $\Phi_i$  is the initial bound  $S$ -state wave function with  $l_i = 0$ , and  $\Psi_{l_f}$  is the final continuum wave function of the outgoing electron with the momentum  $k$ ,

**Table II.** Phase shift  $\eta$  (radians) for e-C<sup>5+</sup>, and e-O<sup>7+</sup> scattering

$k$	C <sup>5+</sup> , <sup>3</sup> P	C <sup>5+</sup> , <sup>1</sup> P	O <sup>7+</sup> , <sup>3</sup> P	O <sup>7+</sup> , <sup>1</sup> P
0.2	8.9261(-2)	-2.7999(-2)	6.7615(-2)	-2.1135(-2)
0.3	8.9269(-2)	-2.7989(-2)	6.7664(-2)	-2.1096(-2)
0.4	8.9019(-2)	-2.8075(-2)	6.7359(-2)	-2.1378(-2)
0.5	8.9084(-2)	-2.7794(-2)	6.7201(-2)	-2.1468(-2)
0.9	8.8104(-2)	-2.7859(-2)	6.6692(-2)	-2.1761(-2)
1.0	8.7596(-2)	-2.7638(-2)	6.5473(-2)	-2.2661(-2)
1.5	8.7811(-2)	-2.5796(-2)	6.6799(-2)	-2.0329(-2)
1.8	8.6016(-2)	-2.5468(-2)	6.5466(-2)	-2.1335(-2)
2.0	8.5094(-2)	-2.5397(-2)	6.3670(-2)	-2.3025(-2)
2.3	8.0013(-2)	-2.2199(-2)	6.4131(-2)	-1.9613(-2)
2.5	7.9218(-2)	-2.1240(-2)	6.6152(-2)	-1.7841(-2)
2.8	8.5047(-2)	-1.9759(-2)	6.5467(-2)	-1.7314(-2)
3.2	8.3225(-2)	-1.7858(-2)	6.4082(-2)	-1.6868(-2)
3.3	8.2661(-2)	-1.7494(-2)	6.3602(-2)	-1.6835(-2)
3.5	8.1361(-2)	-1.7190(-2)	6.2453(-2)	-1.6930(-2)

and  $\omega$  is the energy of the incident photon:

$$\omega = I + k^2, \tag{2.2}$$

$I$  is the ionization potential of the system absorbing the photon, and  $k^2$  is the energy of the photoelectron, and they are in Rydberg units (cf. Appendix A for the derivation of Eq. (2.1)).

We use here the length form for the cross section because this form is the most suitable when the long-range correlations are included in the final-state wave functions and most of the contributions to the matrix elements in Eq. (2.1) comes from the outer region rather than the region close to the nucleus. We assume in the derivation of Eq. (2.1), the plane-wave normalization. Therefore, we have the coefficient  $4\pi(2l_f + 1)$  in Eq. (2.1).  $\Phi_i$ , the <sup>1,3</sup>S-state wave function of the target, is of the Hylleraas form and is given by

$$\Phi_i(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{8\pi^2}} \sum_{lmn} C_{lmn} \left[ e^{-ar_1-br_2} r_1^l r_2^m r_{12}^n \pm (1 \leftrightarrow 2) \right] \tag{2.3}$$

**Table III.** Convergence of photoionization cross sections (Mb) for the <sup>3,1</sup>S state of Be<sup>2+</sup>, C<sup>4+</sup>, O<sup>6+</sup>

$k$	$N_\omega = 84$	120	165
	Be <sup>2+</sup> , 1s <sup>2</sup> 1S		
0.1	1.2725	1.2725	1.2719
0.3	1.2532	1.2532	1.2526
1.0	1.0575	1.0575	1.0570
2.0	6.4120(-1)	6.4123(-1)	6.4129(-1)
2.8	3.7245(-1)	3.7248(-1)	3.7247(-1)
3.3	2.5595(-1)	2.5597(-1)	2.5606(-1)
	Be <sup>2+</sup> , (1s2s) <sup>1</sup> S		
0.1	1.4510	1.4417	1.4455
0.3	1.3649	1.3550	1.3588
1.0	7.3908(-1)	7.3769(-1)	7.3745(-1)
2.5	9.3409(-2)	9.3110(-2)	9.3340(-2)
3.2	3.7183(-2)	3.7114(-2)	3.7073(-2)
3.3	3.2712(-2)	3.2668(-2)	3.2617(-2)
	Be <sup>2+</sup> , (1s2s) <sup>3</sup> S		
0.1	1.2706	1.2704	1.2711
0.5	1.0850	1.0850	1.0855
1.0	6.9895(-1)	6.9902(-1)	6.9882(-1)
1.5	3.8201(-1)	3.8203(-1)	3.8196(-1)
2.5	1.0158(-1)	1.0158(-1)	1.0158(-1)
2.8	6.8786(-2)	6.8786(-2)	6.8772(-2)
3.2	4.2080(-2)	4.2081(-2)	4.2072(-2)
3.3	3.7188(-2)	3.7189(-2)	3.7182(-2)
	Be <sup>2+</sup> , (1s3s) <sup>3</sup> S		
0.2	1.9982	2.0128	2.0067
0.3	1.8431	1.8559	1.8525
0.5	1.4542	1.4622	1.4631
1.0	6.2701(-1)	6.2474(-1)	6.2572(-1)
	$N_\omega = 56$	84	120
	C <sup>4+</sup> , (1s2s) <sup>3</sup> S		
0.2	5.1079(-1)	5.1091(-1)	5.1122(-1)
0.4	4.9362(-1)	4.9379(-1)	4.9407(-1)
1.8	2.3863(-1)	2.3882(-1)	2.3870(-1)
2.5	1.3586(-1)	1.3578(-1)	1.3579(-1)
3.5	5.8413(-2)	5.8364(-2)	5.8380(-2)

*Table Contd.*

	$N_\omega = 56$	84	120
	$C^{4+}, (1s3s)^3S$		
0.2	8.3726(-1)	8.3540(-1)	8.3710(-1)
0.3	8.1107(-1)	8.0913(-1)	8.1095(-1)
1.8	1.9949(-1)	1.9957(-1)	1.9904(-1)
2.5	8.5205(-2)	8.5053(-2)	8.5021(-2)
	$C^{4+}, (1s^2)^1S$		
0.2	4.8680(-1)	4.8683(-1)	4.8685(-1)
0.3	4.8484(-1)	4.8486(-1)	4.8488(-1)
0.5	4.7977(-1)	4.7977(-1)	4.7979(-1)
0.9	4.5782(-1)	4.5778(-1)	4.5781(-1)
2.0	3.5859(-1)	3.5843(-1)	3.5846(-1)
3.5	2.0457(-1)	2.0454(-1)	2.0453(-1)
	$C^{4+}, (1s2s)^1S$		
0.4	5.3101(-1)	5.2929(-1)	5.2845(-1)
1.5	2.9996(-1)	3.0267(-1)	3.0261(-1)
2.8	1.0257(-1)	1.0262(-1)	1.0273(-1)
$k$	$N_\omega = 84$	120	165
	$O^{6+}, (1s^2)^1S$		
	$N_\omega = 35$	56	84
0.2	2.5339(-1)	2.5328(-1)	2.5326(-1)
0.3	2.5282(-1)	2.5271(-1)	2.5269(-1)
1.0	2.4337(-1)	2.4329(-1)	2.2433(-1)
	$O^{6+}, (1s2s)^1S$		
0.2	2.8495(-1)	2.8619(-1)	2.8614(-1)
0.3	2.8276(-1)	2.8392(-1)	2.8391(-1)
0.9	2.5369(-1)	2.5384(-1)	2.5426(-1)
	$O^{6+}, (1s2s)^3S$		
0.2	2.7255(-1)	2.7160(-1)	2.7191(-1)
0.3	2.7073(-1)	2.6977(-1)	2.7009(-1)
1.0	2.3794(-1)	2.3702(-1)	2.3731(-1)
3.3	7.7414(-1)	7.7547(-1)	7.7485(-1)
	$O^{6+}, (1s3s)^3S$		
0.2	6.0934(-1)	4.5927(-1)	4.5897(-1)
0.3	5.9175(-1)	4.5143(-1)	4.5114(-1)
0.9	4.4786(-1)	3.5706(-1)	3.5686(-1)
1.0	4.1280(-1)	3.3456(-1)	3.3439(-1)
3.2	4.9138(-2)	5.7694(-2)	5.7713(-2)
3.3	4.4972(-2)	5.2324(-2)	5.2339(-2)

**Table IV.** Photoabsorption cross sections (Mb) in the two-electron systems

$k$	Cross sections		
	Be <sup>2+</sup> , (1s2s) <sup>3</sup> S	C <sup>4+</sup> , (1s2s) <sup>3</sup> S	O <sup>6+</sup> , (1s2s) <sup>3</sup> S
0.1	1.2711		
0.2	1.2457	5.1122(-1)	2.7191(-1)
0.3	1.2047	5.0358(-1)	2.7009(-1)
0.4	1.1505	4.9407(-1)	2.6741(-1)
0.5	1.0855	4.8203(-1)	2.6397(-1)
0.9	7.7643(-1)	4.1516(-1)	2.4341(-1)
1.0	6.9882(-1)	3.9559(-1)	2.3731(-1)
1.5	3.8196(-1)	2.9419(-1)	1.9961(-1)
1.8	2.5859(-1)	2.3870(-1)	1.7596(-1)
2.0	1.9789(-1)	2.0521(-1)	1.6404(-1)
2.5	1.0158(-1)	1.3579(-1)	1.2358(-1)
2.8	6.877(-2)	1.0536(-1)	1.0455(-1)
3.2	4.2072(-2)	7.6111(-2)	8.2481(-1)
3.3	3.7182(-2)	6.9533(-2)	7.7485(-1)
3.5	2.8930(-2)	5.8380(-2)	6.8620(-1)
	Be <sup>2+</sup> , (1s3s) <sup>3</sup> S	C <sup>4+</sup> , (1s3s) <sup>3</sup> S	O <sup>6+</sup> , (1s3s) <sup>3</sup> S
0.2	2.0067	8.3710(-1)	4.5897(-1)
0.3	1.8525	8.1095(-1)	4.5114(-1)
0.4	1.6642	7.7657(-1)	4.4028(-1)
0.5	1.4631	7.3512(-1)	4.2743(-1)
0.9	7.5586(-1)	5.3996(-1)	3.5686(-1)
1.0	6.2572(-1)	4.9175(-1)	3.3439(-1)
1.5	2.4208(-1)	2.8164(-1)	2.4064(-1)
1.8	1.4027(-1)	1.9904(-1)	1.8968(-1)
2.0	9.7432(-2)	1.5569(-1)	1.6098(-1)
2.5	4.2597(-2)	8.5021(-2)	1.0390(-1)
2.8	2.6904(-2)	5.9954(-2)	7.9761(-2)
3.2	1.5311(-2)	3.8682(-2)	5.7713(-2)
3.3	1.3577(-2)	3.5111(-2)	5.2339(-2)
3.5	1.0083(-2)	2.8330(-2)	4.4013(-2)

*Table Contd.*

$k$	Cross sections		
	Be <sup>2+</sup> , 1s <sup>2</sup> 1S	C <sup>4+</sup> , 1s <sup>2</sup> 1S	O <sup>6+</sup> , 1s <sup>2</sup> 1S
0.1	1.2719		
0.2	1.2634	4.8685(-1)	2.5326(-1)
0.3	1.2526	4.8488(-1)	2.5269(-1)
0.4	1.2362	4.8222(-1)	2.5200(-1)
0.5	1.2148	4.7979(-1)	2.5105(-1)
0.9	1.0956	4.5781(-1)	2.4497(-1)
1.0	1.0570	4.5094(-1)	2.4226(-1)
1.5	8.5066(-1)	4.0852(-1)	2.2971(-1)
1.8	7.2393(-1)	3.7919(-1)	2.2046(-1)
2.0	6.4129(-1)	3.5846(-1)	2.1404(-1)
2.5	4.6127(-1)	3.0395(-1)	1.9374(-1)
2.8	3.7247(-1)	2.7238(-1)	1.8582(-1)
3.2	2.7329(-1)	2.3207(-1)	1.6516(-1)
3.3	2.5606(-1)	2.2268(-1)	1.6109(-1)
3.5	2.1938(-1)	2.0453(-1)	1.5301(-1)
	Be <sup>2+</sup> , (1s2s) <sup>1</sup> S	C <sup>4+</sup> , (1s2s) <sup>1</sup> S	O <sup>6+</sup> , (1s2s) <sup>1</sup> S
0.1	1.4455		
0.2	1.4120	5.4786(-1)	2.8614(-1)
0.3	1.3588	5.3962(-1)	2.8391(-1)
0.4	1.2890	5.2845(-1)	2.8090(-1)
0.5	1.2060	5.1526(-1)	2.7701(-1)
0.9	8.2772(-1)	4.3736(-1)	2.5426(-1)
1.0	7.3745(-1)	4.1490(-1)	2.4745(-1)
1.5	3.8160(-1)	3.0261(-1)	2.0614(-1)
1.8	2.5071(-1)	2.4174(-1)	1.8059(-1)
2.0	1.8833(-1)	2.0596(-1)	1.6413(-1)
2.5	9.3340(-2)	1.3406(-1)	1.2461(-1)
2.8	6.2076(-2)	1.0273(-1)	1.0464(-1)
3.2	3.7073(-2)	7.2424(-2)	8.1447(-2)
3.3	3.2617(-2)	6.6285(-2)	7.6337(-2)
3.5	2.5196(-2)	5.5330(-2)	6.8218(-2)

**Table V.** Recombination rate coefficients (cm<sup>3</sup>/s) for (1s<sup>2</sup>)<sup>1</sup>S states of Be<sup>2+</sup>, C<sup>4+</sup>, and O<sup>6+</sup>

$T(K)$	$\alpha_{R \times 10^{13}}, \text{Be}^{2+}$	$\alpha_{R \times 10^{12}}, \text{C}^{4+}$	$\alpha_{R \times 10^{13}}, \text{O}^{6+}$
1000	16.83	10.92	1.13
2000	16.12	10.42	9.69
5000	12.52	8.09	24.47
7000	11.29	7.28	28.14
10000	10.28	6.61	31.25
12000	9.83	6.31	32.24
15000	9.25	5.93	32.81
17000	8.89	5.69	32.50
20000	8.36	5.35	31.68
22000	8.03	5.13	30.97
25000	7.57	4.83	29.84
30000	6.91	4.40	27.86
35000	6.37	4.04	26.10
40000	5.93	3.75	24.61

**Table VI.** Recombination rate coefficients (cm<sup>3</sup>/s) for (1s2s)<sup>3</sup>S states of Be<sup>2+</sup>, C<sup>4+</sup>, and O<sup>6+</sup>

$T(K)$	$\alpha_{R \times 10^{13}}, \text{Be}^{2+}$	$\alpha_{R \times 10^{14}}, \text{C}^{4+}$	$\alpha_{R \times 10^{14}}, \text{O}^{6+}$
1000	2.67	1.09	2.12
2000	2.55	9.39	18.18
5000	1.99	23.78	46.06
7000	1.80	27.34	53.97
10000	1.64	30.34	58.79
12000	1.57	31.37	60.79
15000	1.48	31.82	61.60
17000	1.43	31.60	61.24
20000	1.34	30.82	59.72
22000	1.29	30.13	58.38
25000	1.22	28.99	56.18
30000	1.11	27.12	52.56
35000	1.03	25.44	49.31
40000	0.96	24.00	46.50

**Table VII.** S state energies for Be<sup>2+</sup>, C<sup>4+</sup>, and O<sup>6+</sup> for various number of terms

System	State	$a$	$B$	$N_\omega$	$E(Ry)$
Be <sup>2+</sup>	(1s <sup>2</sup> ) <sup>1</sup> S	4.30	5.75	84	-27.3111313
		5.00	5.75	120	-27.3111328
		4.80	5.74	165	-27.3111392
Be <sup>2+</sup>	(1s2s) <sup>1</sup> S	1.92	5.61	84	-18.3697337
		2.14	5.24	120	-18.3697441
		2.32	5.11	165	-18.3697468
Be <sup>2+</sup>	(1s2s) <sup>3</sup> S	2.08	4.47	84	-18.5943332
		2.10	4.47	120	-18.5943332
		2.20	4.43	165	-18.5943332
Be <sup>2+</sup>	(1s3s) <sup>3</sup> S	1.20	4.20	84	-17.0939436
		1.20	4.80	120	-17.0939440
		1.20	5.20	165	-17.0939441
C <sup>4+</sup>	(1s <sup>2</sup> ) <sup>1</sup> S	8.70	5.88	56	-64.8124875
		9.50	6.10	84	-64.8124917
		9.90	6.40	120	-64.8124927
C <sup>4+</sup>	(1s2s) <sup>1</sup> S	6.68	3.24	56	-42.4439868
		7.41	3.35	84	-42.4440237
		8.05	3.37	120	-42.4440313
C <sup>4+</sup>	(1s2s) <sup>3</sup> S	4.00	4.50	56	-42.8415115
		3.90	5.30	84	-42.8415118
		3.90	5.40	120	-42.8415118
C <sup>4+</sup>	(1s3s) <sup>3</sup> S	6.20	1.90	56	-38.9408051
		6.00	2.00	84	-38.9408055
		6.20	2.20	120	-38.9408060
O <sup>6+</sup>	(1s <sup>2</sup> ) <sup>1</sup> S	10.90	7.80	35	-118.3131656
		11.70	7.80	56	-118.3131841
		12.50	8.10	84	-118.3131886
O <sup>6+</sup>	(1s2s) <sup>1</sup> S	3.94	9.00	35	-76.5172983
		4.12	10.10	56	-76.5174612
		4.50	10.10	84	-76.5175009
O <sup>6+</sup>	(1s2s) <sup>3</sup> S	3.20	9.50	35	-77.0892922
		3.80	9.50	56	-77.0892944
		4.20	9.30	84	-77.0892946
O <sup>6+</sup>	(1s3s) <sup>3</sup> S	3.39	7.20	35	-69.6726623
		2.68	8.25	56	-69.6768186
		2.66	8.45	84	-69.6768189

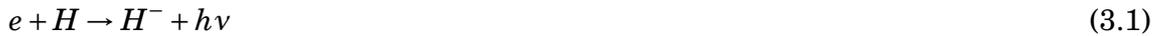
The distance between the two electrons is given by  $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ . The upper sign in Eq. (2.3) refers to the singlet state and the lower sign refers to the triplet state. The minimum value of  $l$ ,  $m$ , and  $n$  are 0. The nonlinear parameters are  $a$  and  $b$ , and  $C_{lmn}$  are the eigenvectors. Energies for various number of terms are given in Table VII in the Appendix B for Be<sup>2+</sup>, C<sup>4+</sup> and O<sup>6+</sup> ions. The cross section has a finite value for  $k \rightarrow 0$  which is due to the fact that the final-state function is a Coulomb function and, therefore,  $u(r) \propto 1/\sqrt{k}$ , and the expression for the cross section becomes independent of  $k$ , the outgoing photoelectron momentum.

In Table III, we show the convergence of the photoionization cross sections for a few values of the outgoing electron momentum  $k$  for the triplet and singlet ground and excited states of three ions with respect to various number of terms in the bound state function. It is seen that in most cases the cross sections have converged very well.

In Table IV, we give the photoabsorption cross sections for the maximum number of terms for the ion. We find that the cross sections for the excited states are always larger than those for the ground state.

### 3. Radiative Attachment

Radiative attachment played an important role in the formation of molecules when in the early universe temperature of matter and radiation dropped to a few thousand degrees. Such processes are of the form:



These processes are exothermal processes and the radiative recombination cross section is small compared to the photoabsorption cross sections. The attachment cross section  $\sigma_a$  is obtained by using the principle of detailed balance and is given by

$$\sigma_a = \left( \frac{h\nu}{cp_e} \right)^2 \frac{g(f)}{g(i)} \sigma = \left( \frac{h\nu}{c} \right)^2 \frac{1}{2mE} \frac{g(f)}{g(i)} \sigma. \quad (3.3)$$

In the above expression,  $p_e = k$  is the momentum of the incident electron. The radiative rate coefficient, obtained by averaging over the Maxwellian velocity distribution  $f(E)$ , is given by

$$\alpha_R(T) = \langle \sigma_a v_e f(E) \rangle. \quad (3.4)$$

The electron velocity is given by  $v_e$  and the Maxwellian distribution is given by

$$f(E)dE = \sqrt{\frac{4}{\pi}} \frac{1}{(k_B T)^{3/2}} \sqrt{E} e^{-E/k_B T}. \quad (3.5)$$

The rate coefficient is given by

$$\alpha_R(T) = \sqrt{2/\pi} \frac{c}{(mc^2 k_B T)^{1.5}} \frac{g(f)}{g(i)} \int_0^\infty dE (E+I)^2 \sigma e^{-E/k_B T}, \quad (3.6)$$

where  $E = k^2$  is the energy of the electron,  $k_B$  is the Boltzmann constant,  $T$  is the electron temperature and  $h\nu = E + I$  where  $I$  is the threshold for photoionization. Considering the

spin states of the electron, the angular momentum, and the polarization directions of the electromagnetic field, we have  $g(i) = 4(2l_i + 1)$ , where  $l_i = 1$  and  $g(f) = 6(2S + 1)$ , where  $S$  is the spin of the final state of the combined ion. Substituting the values of various quantities, the above expression can be written as

$$\alpha_R(T) = (2S + 1)10.2509x10^{10} \int_0^\infty dE(E + I)^2 \sigma(E)e^{-E/k_B T}. \quad (3.7)$$

The photoionization cross section  $\sigma(E)$  in Eq. (3.7) is in units of Mb. We have calculated the radiative attachment to Be<sup>2+</sup>, C<sup>4+</sup>, and O<sup>6+</sup> for the lowest singlet and triplet states at various temperatures. The rate coefficients for the singlet states are given in Table V and for the triplet states in Table VI. Most of the contribution to the integral comes from the first few energy points. In general, the rate coefficients decrease with the increase of electron temperature.

### 4. Fitting Formulae

Cross sections have not been calculated at every possible value of the photoelectron momentum  $k$ . Therefore, fitting formulae are given here for interpolation to calculate cross section at any desired value of  $k$ . The fitting formulae are given for the singlet and triplet states of Be<sup>2+</sup>, C<sup>4+</sup>, and O<sup>6+</sup>:

Be<sup>2+</sup>

$$\sigma(1s^2^1S) = 2.60168 - 1.14545k + 0.137894k^2 - 1.33351e^{-0.905k}$$

$$\sigma(1s2s^1S) = -1.46694 + 0.69944k - 0.08841k^2 + 5.943316e^{-1.1k} - 3.05516e^{-2.064k}$$

$$\sigma(1s2s^3S) = -3.251195 + 1.324675k - 0.1486286k^2 - 1.888434e^{-2.03k} + 6.3905e^{-0.75k}$$

$$\sigma(1s3s^3S) = -0.339773 + 0.185816k - 0.025689k^2 - 1.77079e^{-5.2k} + 4.072009e^{-1.6k}$$

C<sup>4+</sup>

$$\sigma(1s^2^1S) = 1.133578 - 0.32748k + 0.026087k^2 - 0.64639e^{-0.525k}$$

$$\sigma(1s2s^1S) = 1.557819 - 0.68380k + 0.0832431k^2 - 0.973418e^{-0.579k}$$

$$\sigma(1s2s^3S) = 1.434879 - 0.69133k + 0.092088k^2 - 0.90868e^{-0.723k}$$

$$\sigma(1s3s^3S) = -3.08341 + 1.181578k - 0.12042k^2 + 5.296694e^{-0.66k} - 1.377198e^{-1.84k}$$

O<sup>6+</sup>

$$\sigma(1s^2^1S) = 0.275206 - 0.021982k - 0.0037533k^2 - 0.0203266e^{-1.1k} - 0.00279897e^{-4k}$$

$$\sigma(1s2s^1S) = 0.442368 - 0.170170k - 0.01812097k^2 - 0.1758088e^{-1.4k} - 0.0240454e^{-4.4k}$$

$$\sigma(1s2s^3S) = 0.4422471 - 0.15579k + 0.015711k^2 - 0.16747e^{-1.3k} - 0.020087e^{-3.9k}$$

$$\sigma(1s2s^3S) = -1.619851 + 0.534168k - 0.0484744k^2 + 6.733557e^{-0.7k} - 4.654739e^{-0.91k}$$

## 5. Conclusions

The long-range potential has been included in the scattering equation variationally and therefore the present results for the phase shifts have lower bounds to the exact phase shifts. The present approach is applied to calculate photoionization cross sections of the singlet and triplet states of Be<sup>2+</sup>, C<sup>4+</sup>, and O<sup>6+</sup>. The photoionization cross sections calculated here for various excited states would be useful in the investigations of the solar and stellar objects. These cross sections are further used to calculate the Maxwellian-averaged radiative attachment rate coefficients at various electron temperatures, the recombined states being <sup>1,3</sup>S states of Be<sup>2+</sup>, C<sup>4+</sup>, and O<sup>6+</sup>. These rates decrease with the increase of the electron temperature.

As for the accuracy of the calculations, all phase shifts and cross sections have converged to better than the third decimal place.

## Appendix A

Cross section expression for photoionization is well known. However, it would be instructive to describe briefly the derivation by considering the photoionization process of the hydrogen atom:

$$h\nu + H \rightarrow H^+ + e. \quad (\text{A.1})$$

The interaction Hamiltonian is given by

$$H' = -\frac{e}{2mc}(\vec{A} \cdot \vec{p} + \vec{p} \cdot \vec{A}) = -\frac{e}{mc}\vec{A} \cdot \vec{p}, \quad (\text{A.2})$$

where  $\mathbf{p}$  is the electron momentum and  $A$  is the vector potential with the condition that  $\text{div } \vec{A} = 0$ , and it can be represented by

$$\vec{A} = A_0 \hat{e} e^{i\vec{k} \cdot \vec{r}}. \quad (\text{A.3})$$

In the above equation  $k_{ph}$  is the photon momentum which is less than the radius  $r$  which implies that the exponential factor is equal to 1, the dipole approximation, and  $\hat{e}$  is the polarization direction, perpendicular to the z-axis, the incident photon direction. The density of states is given by

$$\rho(k) = \frac{mk}{(2\pi)^3 \hbar^2} \sin(\vartheta) d\vartheta d\phi \quad (\text{A.4})$$

Here  $\theta$  is the angle between  $\vec{k}$  and the photon direction z. The incident flux is given by

$$\text{Flux} = \frac{\omega^2 A_0^2}{2\pi c(\hbar\omega)} = \frac{\omega A_0^2}{2\pi \hbar c}. \quad (\text{A.5})$$

The electron momentum satisfies the commutation relation

$$\langle \vec{p} \rangle = m \frac{d\vec{r}}{dt} = m \left\langle \frac{1}{i\hbar} [H, \vec{r}] \right\rangle = \frac{mE}{i\hbar} \langle \vec{r} \rangle = \frac{m\omega}{i} \langle \vec{r} \rangle. \quad (\text{A.6})$$

Therefore,

$$\langle H' \rangle = -\frac{e}{mc} \langle \vec{A} \cdot \vec{p} \rangle = -\frac{e\omega A_0}{ic} \langle \vec{e} \cdot \vec{r} \rangle. \quad (\text{A.7})$$

The transition probability is given by

$$\omega_p = \frac{2\pi}{\hbar} \rho(k) |\langle H' \rangle|^2 = \frac{2\pi}{\hbar} \rho(k) \frac{e^2 \omega^2}{c^2} |A_0|^2 |\langle \vec{\epsilon} \cdot \vec{r} \rangle|^2 \quad (\text{A.8})$$

Since

$$\hat{\epsilon} \cdot \hat{r} = P_1(\hat{\epsilon} \cdot \hat{k}) P_1(\hat{k} \cdot \hat{r}), \quad (\text{A.9})$$

we get,

$$\sigma(\vartheta, \phi) \sin(\vartheta) d\vartheta d\phi = \frac{\omega_p}{Flux} = \frac{1}{2\pi} \frac{mk}{\hbar^2} \frac{e^2 \omega}{c} |\langle \vec{k} \cdot \vec{r} \rangle|^2 \sin^3(\vartheta) \cos^2(\phi) d\vartheta d\phi. \quad (\text{A.10})$$

Integration over angles gives  $4\pi/3$ . Therefore, the total cross section is

$$\sigma = \frac{2m}{\hbar^2} \frac{e^2}{\hbar c} k \frac{\hbar \omega}{3} |\langle \vec{k} \cdot \vec{r} \rangle|^2. \quad (\text{A.11})$$

Now,  $e^2/\hbar c = \alpha$ , the fine-structure constant,  $2m/\hbar^2 = 1/(Ry a_0^2)$ , and  $\hbar \omega = E = I + k^2$ , where  $I$  is the ionization potential and  $k$  is the momentum of the photoelectron. We get the photoabsorption cross section in units of  $a_0^2$  with  $I + k^2$  in  $Ry$  units,

$$\sigma = \frac{\alpha k}{3} (I + k^2) |\langle \hat{k} \cdot \vec{r} \rangle|^2. \quad (\text{A.12})$$

If we choose  $k$  in the  $z$ -direction, then  $\hat{k} \cdot \vec{r} = r \cos(\theta) = z$  and the cross section is given by

$$\sigma = \frac{\alpha k}{3} (I + k^2) |\langle \Psi_f | z | \Phi \rangle|^2. \quad (\text{A.13})$$

In the above equation,  $\Phi$  is the bound state wave function with angular momentum equal to 0 and  $\Psi_f$  is the final state continuum function with angular momentum equal to 1. If use the plane wave normalization, then in the asymptotic region

$$\Psi_f = \sqrt{12\pi} j_1(kr) Y_{10}(\theta). \quad (\text{A.14})$$

The total photoabsorption cross section is given by

$$\sigma = 4\pi \alpha k (I + k^2) |\langle \Psi'_f | z | \Phi \rangle|^2, \quad (\text{A.15})$$

and

$$\Psi'_f = j_1(kr) Y_{10}(\theta). \quad (\text{A.16})$$

The above expression for the cross section can be generalized to any initial angular momentum state and for any number of electrons in the target.

## Appendix B

In Table VII, we give nonlinear parameters and energies of various  $1,3S$  states of  $Be^{2+}$ ,  $C^{4+}$ , and  $O^{6+}$  for a number of terms in the Hylleraas function, Eq. (2.3). All energies have converged to six or seven decimal places when the number of terms is increased to the highest number of terms in the expansion.

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## Competing Interests

The author declare that they have no competing interests.

## Authors' Contributions

Author contributed significantly in writing this article. The author read and approved the final manuscript.

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