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Electron impact rotational excitation cross section of an astronomically important molecular ion with a large dipole moment: PO^+

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PAPER

Electron impact rotational excitation cross section of an astronomically important molecular ion with a large dipole moment: PO⁺

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E-mail: jasmeet.singh@keshav.du.ac.in**Keywords:** electron–molecule collision, spectral data, atmospheres-planets, atmospheres-ISM, clouds-ISMSupplementary material for this article is available [online](#)**Abstract**

The phosphorus monoxide ion (PO⁺) has a permanent dipole moment of about 4 debyes; it has been detected in space with a higher abundance relative to neutral PO than other comparable species. However, rotational excitation cross sections are needed to confirm these abundance estimates. Rotational excitation cross sections and rates for electron collisions with PO⁺ are computed using the UK *R*-matrix method and multichannel quantum defect theory. The scattering matrices generated from the UK *R*-matrix method are used as the input to compute cross-sections, then the channel elimination procedure is applied to study spectroscopy in the microwave region. We determine that the $\Delta j = 2$ excitation rates dominate over $\Delta j = 1$ rates for both excitation and de-excitation processes. We reported a number of resonances in ²Δ, ²Π and ²Σ⁺ symmetries of the e-PO⁺ system. Electron impact electronic excitation and ionization cross sections are also provided.

1. Introduction

Any molecule must have an asymmetric charge distribution that gives a permanent dipole moment (μ) to undergo a rotation transition. The strength of the rotational transition depends on μ^2 , therefore molecules with large permanent dipoles have intense transitions (Tennyson 2019). Large dipoles therefore greatly aid the astronomical detection of such species even at low column densities. Molecular ions are particularly important because they have electron impact rotational excitation cross sections many orders of magnitude greater than those given by neutral molecule collisions (Faure and Tennyson 2001); given that interstellar species are usually not in thermal equilibrium, there is a direct relationship between collisional excitation rates and observed line emissions.

PO⁺ has been detected in space (Rivilla *et al* 2022) aided by its large dipole moment of about 4 debyes. PO⁺ is a closed shell system and therefore can be expected to be relatively stable. The different properties of PO⁺ ions are of interest in various fields such as astrophysics, quantum chemistry, molecular physics and plasma physics. Studying these types of ions, which have a large dipole moment, can provide insight into chemical reactions in extreme environments and help to understand complex chemical processes in space and in the laboratory (Peterson and Woods 1990, Rivilla *et al* 2022, Qin *et al* 2023).

The ionization potential of phosphorus is lower than nitrogen and sulfur making it easier to form PO⁺ than SO⁺ or the well-studied NO⁺. In the interstellar medium, the PO⁺ to PO ratio in the Universe is significantly higher than that of NO⁺/NO and SO⁺/SO (Rivilla *et al* 2022). PO⁺ molecules are formed when cosmic rays effectively ionize gaseous phosphorus elements, which are created when interstellar ice shells collide. This is followed by interactions with oxygen or hydroxyl radicals. PO⁺ is

thought to play a dominant role in interstellar chemistry compared to other phosphorus-containing compounds due to its higher abundance (Rivilla *et al* 2022).

In a recent theoretical study, Wang *et al* (2025) computed spectral line positions and intensities for PO^+ molecular ions in the ultraviolet and infrared ranges. They combine their partition function with the dipole moment function and the transition dipole moment function of the PO^+ molecule generated through a multi-reference configuration interaction method. Using computed results they determined the Einstein coefficients for the $X^1\Sigma^+$ state and $X^1\Sigma^+ \leftrightarrow C^1\Pi$ transitions; and spectral intensities at two different temperatures (296 K and 3000 K). Further related references are given by Moussaoui *et al* (2003), Wang *et al* (2025) and Metropoulos *et al* (2003).

The present study computes the low energy electron impact excitation cross section, rotational excitation cross sections with rate coefficients, excitation energy energies and resonance parameters for PO^+ .

2. Computational details

2.1. R-matrix method

The UK *R*-matrix method (Tennyson 2010) is used to study electron–molecule scattering, generate scattering matrices and as an input to compute rotational excitation cross-sections. This method divides the space around the target system into two parts: the inner region and the outer region. The wave function associated with the target molecule is contained within the inner region (Tennyson 2010). The energy of incoming electron is not considered in inner region scattering calculations, however it is used in solving the outer region problem in a simple and fast way. This makes the method more useful for studying complicated systems with many resonances which have energy dependence. In the present case of electron scattering with positively charged molecular ions, these two advantages make the *R*-matrix method efficient for studying the system having compact target wave functions and complicated resonance structures.

In the inner region, the wave function of the target (PO^+) and a single continuum electron, together having $N+1$ electrons, is taken as

$$\Psi_k = \mathcal{A} \sum_{i,j} a_{i,j,k} \Phi_i(1, \dots, N) F_{i,j}(N+1) + \sum_i b_{i,k} \chi_i(1, \dots, N+1) \quad (1)$$

where $\mathcal{A}$ is an anti-symmetrization operator, $\Phi_i(1, \dots, N)$ is the wave function of the N electron target and $F_{i,j}(N+1)$ are continuum orbitals. The functions $\chi_i(1, \dots, N+1)$ in the last term are called square integrable functions, responsible for electrons entering the target complete active space (CAS) and are included to take into account electron correlations and polarization of the target in the presence of the projectile electrons. The coefficients $a_{i,j,k}$ and $b_{i,k}$ are obtained by diagonalizing the inner region Hamiltonian (Tennyson 1996).

The inner region wave function Ψ_k in equation (1) is then used with appropriate boundary conditions to construct scattering energy-dependent *R*-matrices on the boundary which are then propagated to large distances to give scattering information. Details of our calculations are given in the following subsections.

2.2. Scattering calculations

A cc-pVTZ Gaussian type orbital basis set is used to represent the PO^+ target in the scattering calculations. A CAS configuration interaction (CAS-CI) wave-function expansion is used in the inner region with nine target states lying below 10 eV. The molecular ion PO^+ is a linear system with ground state $X^1\Sigma^+$ in the $C_{\infty v}$ point group which is projected to the C_{2v} point group when the symmetry is lowered. The Hartree–Fock electronic configuration for the ground state is $(1\sigma)^2(2\sigma)^2(3\sigma)^2(4\sigma)^2(1\pi)^4(5\sigma)^2(6\sigma)^2(2\pi)^4(7\sigma)^2$. In the present CAS-CI model, twelve electrons were kept frozen in $(1\sigma)^2(2\sigma)^2(3\sigma)^2(4\sigma)^2(1\pi)^4$ and the remaining ten electrons were allowed to move freely in $(5\sigma)(6\sigma)(2\pi)(7\sigma)(8\sigma)(3\pi)$ molecular orbitals. The ground state energy of the PO^+ with dipole moment at equilibrium bond length of 1.469 Å given in table 1 for close-coupling (CC) calculation.

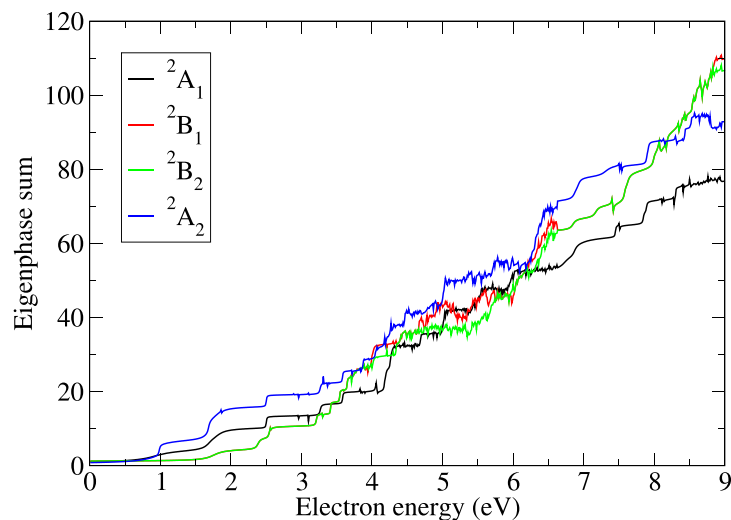
Our CC calculation uses an expansion of the nine lowest electronic states of PO^+ . Table 2 compares the electronic excitation energies of these states with the previous calculations of Wang *et al* (2025) with eight target states. The results are generally in good agreement; the only significant difference with the work of Wang *et al* (2025) is in the order of two states ($^3\Pi$ and $^3\Delta$), our $^3\Pi$ state lie above the $^3\Delta$ state.

Table 1. Comparison of the *R*-matrix calculations with data in literature, dipole moment (μ) and ground state energy (E).

	Present calculations	Theoretical
E/E_h	−415.185 916	−415.679 523 (Frisch <i>et al</i> 2003) −415.733 08 (Metropoulos <i>et al</i> 2003)
μ/D	4.174	4.02 (Frisch <i>et al</i> 2003) 3.44 (Peterson and Woods 1990) 3.13 (Rivilla <i>et al</i> 2022)

Table 2. Vertical electronic excitation energy in eV and the dipole moment at the PO^+ equilibrium geometry (bond length, $r_e = 1.469$ Å) for 9 state CC model. A comparison shown with previous calculation (Wang *et al* 2025).

Target state $C_{\infty v}(C_{2v})$	Present results	Theoretical Wang <i>et al</i> (2025)
X $^1\Sigma^+(^1A_1)$	0	0
a $^3\Sigma^+(^3A_1)$	4.74	4.24
b $^3\Pi(^3B_1/^3B_2)$	5.34	5.22
c $^3\Delta(^3A_1/^3A_2)$	5.43	4.85
d $^3\Sigma^-(^3A_2)$	5.75	5.25
A $^1\Sigma^-(^1A_1)$	5.97	5.30
B $^1\Delta(^1A_1/^1A_2)$	6.02	5.42
C $^1\Pi(^1B_1/^1B_2)$	6.63	6.23
2 $^3\Pi(^3B_1/^3B_2)$	8.95	—

**Figure 1.** Eigenphase sum for electron collisions with PO^+ showing the many resonance features detected by the calculation.

3. Results and discussion

Eigenphase sums of all four symmetries are given in figure 1 for electron collisions with PO^+ . Several peaks are observed in each symmetry due to the interaction of positively charged molecular ions with electrons. A jump of π in eigenphase sum is a key indicator for the presence of resonance.

3.1. Elastic and Excitation cross sections

In figure 2 the excitation cross sections for the first four excited states are presented. The resonances above the first excitation threshold ($^3\Sigma^+$ at 4.74 eV) have a clear presence in the cross sections of all four transitions.

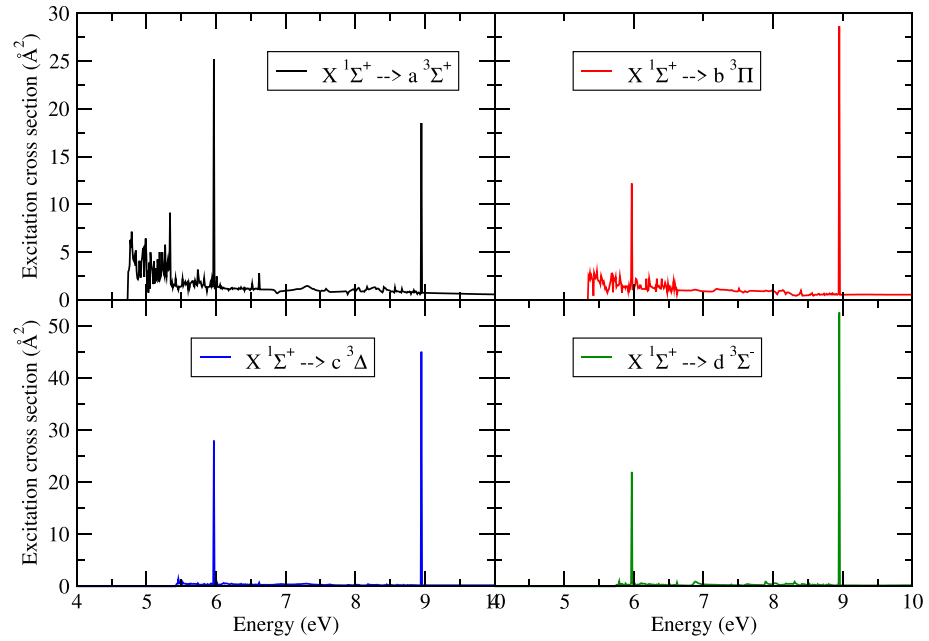


Figure 2. Electronic excitation cross section for the four lowest electronic states of PO^+ .

Table 3. Resonance parameters (in eV) give by the 9 state CC model for $^2\Delta$ ($^2A_1/2A_2$), $^2\Pi$ ($^2B_1/2B_2$) and $^2\Sigma^+$ (2A_1) symmetries of the e- PO^+ system. These resonances lying above ground state ($X\ ^1\Sigma^+$) and below first excited state ($a\ ^3\Sigma^+$) of PO^+ .

Symmetry	Position (E_r)	Width (Γ_r)
$^2\Delta$ ($^2A_1/2A_2$)	0.9849	0.0245
$^2\Delta$ ($^2A_1/2A_2$)	1.6837	0.0297
$^2\Pi$ ($^2B_1/2B_2$)	1.7590	0.2320
$^2\Sigma^+$ (2A_1)	1.8641	0.0046
$^2\Pi$ ($^2B_1/2B_2$)	2.3860	0.0566
$^2\Delta$ ($^2A_1/2A_2$)	2.5014	0.0125
$^2\Pi$ ($^2B_1/2B_2$)	2.5620	0.0285
$^2\Sigma^+$ (2A_1)	2.8912	0.0006
$^2\Pi$ ($^2B_1/2B_2$)	3.2090	0.0194
$^2\Pi$ ($^2B_1/2B_2$)	3.2970	0.0398

3.2. Resonance parameters

Resonances were detected by the characteristic change in the sign of the second derivative of the eigenphase sum $\delta(E)$ given by

$$\delta(E) = \sum_i \arctan(K_{ii}), \quad (2)$$

where K_{ii} are the diagonal elements of the K matrix. They were then fitted to a Breit–Wigner profile (Tennyson and Noble 1984) with an energy grid of 0.01 eV to obtain the resonance energy E and width Γ . The fitted resonance parameters are reported in table 3, resonance position (E_r in eV) and width (Γ in eV). Some resonances for $^2\Delta$ ($^2A_1/2A_2$), $^2\Pi$ ($^2B_1/2B_2$) and $^2\Sigma^+$ (2A_1) symmetries of the e- PO^+ system are tabulated in this table. A complete set of resonance fits for all scattering symmetries is given in the supplementary data.

3.3. Ionization cross sections

The ionization cross section is computed directly by using the binary-encounter Bethe (BEB) model (Kim and Rudd 1994). The orbital energies and kinetic energies produced from Quantemol Electron

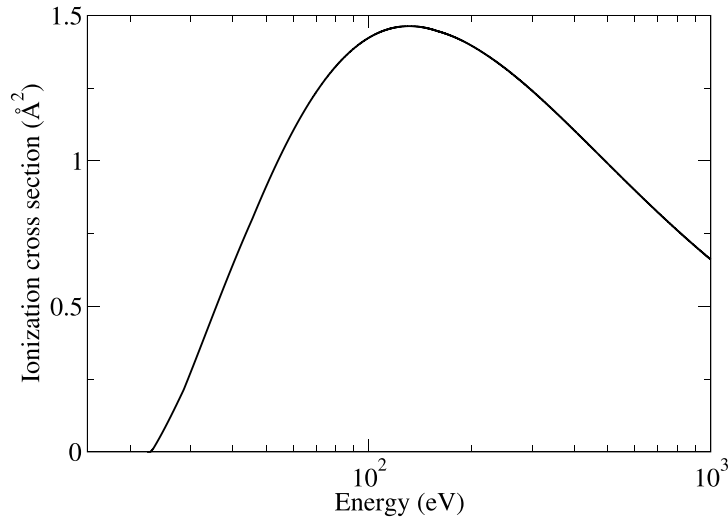


Figure 3. Electron impact ionization cross section for PO^+ .

Collision (QEC) are used for this computation. According to BEB, the cross section σ_{BEB} is given by,

$$\sigma_{\text{BEB}} = \frac{S}{t+u+1} \left[\frac{1}{2} \left(1 - \frac{1}{t^2} \right) \ln t + 1 - \frac{1}{t} - \frac{\ln t}{1+t} \right], \quad (3)$$

where $t = T/B$, $u = U/B$, and $S = 4\pi a_0^2 N(R/B)^2$. a_0 is the Bohr radius, and R is the Rydberg energy. B , U , and N are the binding energy, the average kinetic energy of the bound electron in its orbital, and the occupation number, respectively, for the subshell. If the kinetic energy T of the incident electron is less than B , then $\sigma_{\text{BEB}} = 0$.

The ionization cross section for PO^+ shown in figure 3, the peak of the curve, occurs at 1.46 Å^2 for energy value of 131.14 eV. To our knowledge, no other electron-impact ionization data (experiment or theoretical) for PO^+ are available in the literature for comparison.

3.4. Rotational (de-)excitation cross-sections and rate coefficients

In this method, the UK R -matrix method (Tennyson 2010) combined with multi-channel quantum defect theory (Aymar *et al* 1996, Kokoouline and Greene 2004, Seaton 2019). The QEC expert system (Cooper *et al* 2019), which uses MOLPRO (Werner *et al* 2022) and UK R -matrix method code UKRmol+ (Masin *et al* 2020), was used to generate scattering matrices. The cross-sections and rate coefficients are then computed for different rotation transitions of the target ion, and the detailed method is given in Khamesian *et al* (2018). The cross sections are computed using the following equation (4):

$$\sigma_{j'\mu' \leftarrow j\mu}(E_{el}) = \frac{1}{2j+1} \frac{\pi}{k_j^2} \sum_{J,l,l'} (2J+1) |\delta_{jj'} \delta_{\mu'\mu} \delta_{ll'} - S_{j\mu;j'\mu',l'}^J|^2 \quad (4)$$

here, the S -matrix elements ($S_{j\mu;j'\mu',l'}^J$) are computed under a fixed geometry by applying a frame transformation (lab to body frame) (Kokoouline and Greene 2003) in channel elimination procedure (Aymar *et al* 1996). j and μ represent the angular momentum of PO^+ and its projections, $j\mu$ and $j'\mu'$, are the open and closed channels for ionization, respectively, for a given total energy which is the sum of the energy of the entrance channel E_i and relative kinetic energy E_{el} of electron and target ion: $E = E_i + E_{el}$. The channels having energy lower than the incoming electron are open and the rest having higher energy are called closed channels. We consider that the electron propagates along the z -axis as a plane wave in the laboratory frame having k_j as the wave vector and l as its angular momentum.

In a recent article (Mezei *et al* 2019), a similar methodology (multichannel quantum defect theory and R -matrix) was applied to review the study of dissociative recombination and ro-vibrational excitation of diatomic and small polyatomic molecular ions. They achieved highly accurate results for diatomic systems and reliable results for polyatomic ones.

In the literature, the unphysical behavior of cross-sections at rotational thresholds is corrected using different approaches. This channel elimination procedure is more promising to compute accurate results near rotational thresholds. Figure 4 shows electron-impact rotational (de-)excitation cross-sections for

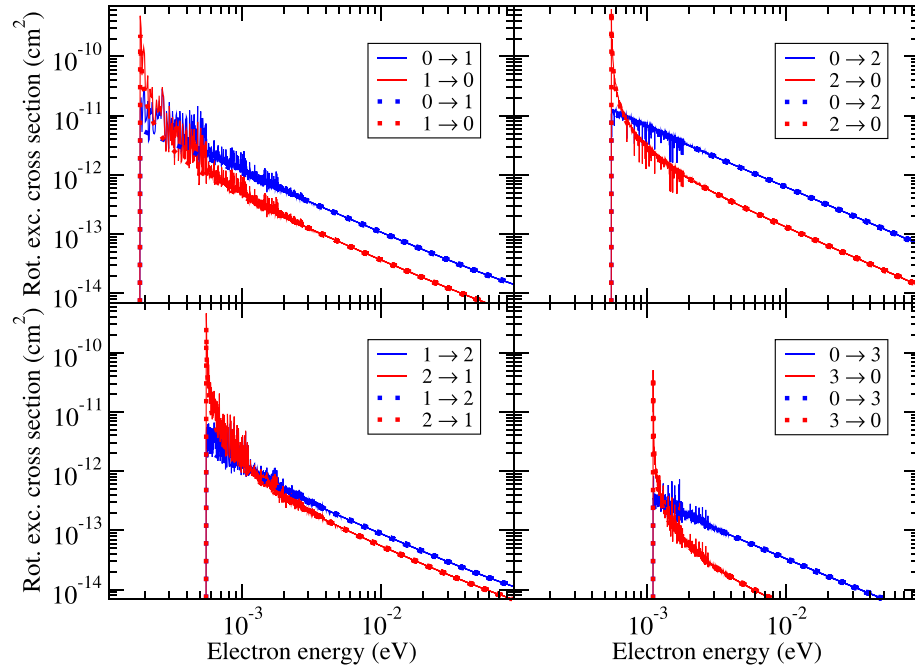


Figure 4. Electron-impact rotational (de-)excitation cross-sections for transitions in four rotational states ($j = 0, 1, 2, 3$) of PO^+ . Solid lines represent frame transformed results. Dotted lines represent results without frame transformation.

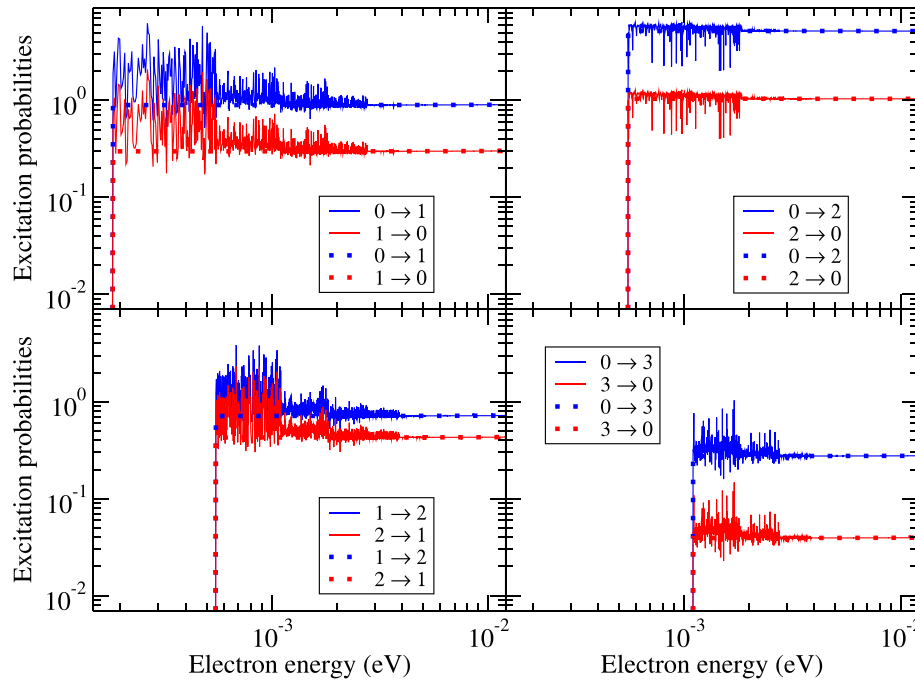


Figure 5. Rotational (de-)excitation probabilities for transitions in four rotational states ($j = 0, 1, 2, 3$) of PO^+ . Solid lines represent frame transformed results. Dotted line represents results without frame transformation.

transitions between the four lowest rotational states of PO^+ . Rotational (de-)excitation probabilities for transitions in four rotational states ($j = 0, 1, 2, 3$) of PO^+ are shown in figure 5. Rate coefficients for transitions from the four rotational states ($j = 0, 1, 2, 3$) of PO^+ are reported in figure 6 for a temperature range from 1 K to 100 000 K. These rates are large at the low electron temperatures important for the interstellar medium. Rate coefficients at 10 000 K are important for plasma modeling and to study high-energy processes like ionization and dissociation which involve emission or capturing of electrons, in stellar atmospheres (Millar and Williams 2012, Fritzsche 2025).

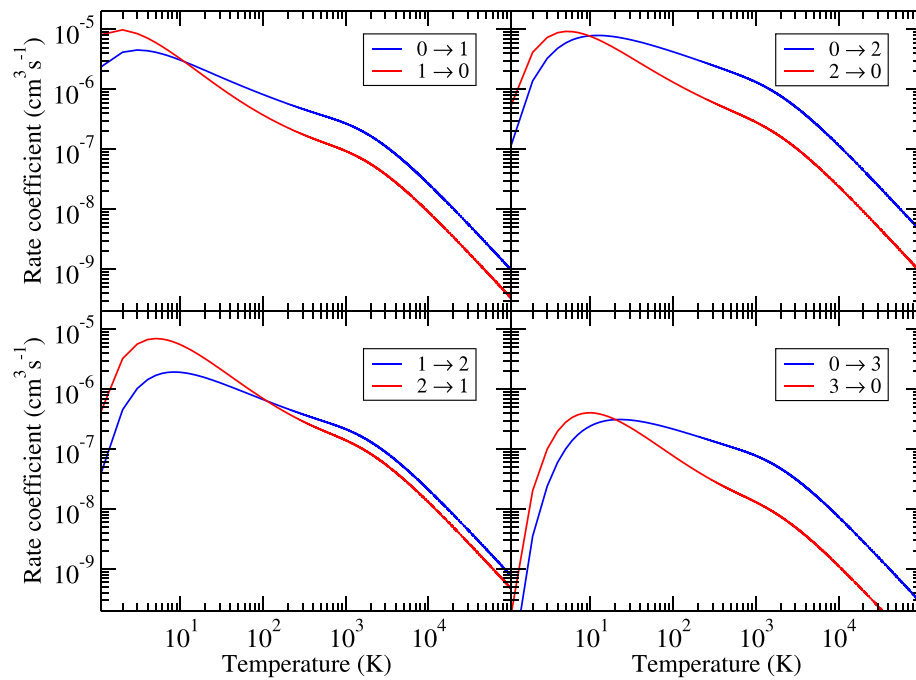


Figure 6. Rate coefficients for transitions from the four rotational states ($j = 0, 1, 2, 3$) of PO^+ for a temperature range from 1 K to 100 000 K.

We note that while a simple Coulomb–Born model, which is based on a Born approximation treatment of the long range interaction between the scattering electron represented by a Coulomb wave and the target dipole (Chu and Dalgarno 1974), would predict large rates for $\Delta j = 1$ processes, we find that excitations with $\Delta j = 2$ are also fast, contrary to predictions of this model. Similar results were found for electron impact rotational excitation of NO^+ (Rabadan *et al* 1998) where it was shown that excitations with $\Delta j > 1$ are largely due to short-range effects not considered in the Coulomb–Born approach.

The effect that transitions with $\Delta j = 1$ are dominated by long-range effects while those with $\Delta j > 1$ are caused by short-range interactions appears to be rather general for linear molecular ions (Faure and Tennyson 2001) and is readily understood in terms of the long-range nature of the dipole interaction compared to the much shorter-range scope of all the other, higher-order, interactions. They noticed large excitation rates of HCO^+ and CO^+ for $\Delta j = 1$ in comparison to that of NO^+ (Faure and Tennyson 2001). In contrast, for $\Delta j = 2$ and $\Delta j = 4$ excitations rates were significantly higher than those $\Delta j = 1$ in NO^+ system. Similar results we obtain for PO^+ as shown in figure 6, excitation rates for $\Delta j = 2$ are greater than $\Delta j = 1$ rates for both excitation and de-excitation processes.

In a very recent study by Mukherjee *et al* (2025) for BH^+ , the cross sections for partial waves $l \leq 6$ computed from the T-matrices and supplemented with the Coulomb–Born cross-sections for large l values. They observed that $\Delta j = 1$ transitions driven by dipole transitions are relatively flat. However $\Delta j = 2$ and $\Delta j = 3$ show rapid oscillations due to short range interactions.

4. Conclusion

We have computed cross sections for electron collisions with PO^+ ion. Our calculations suggest that rotational excitation with $\Delta j = 2$ could be important alongside the standard $\Delta j = 1$ dipole driven transition. Our study has identified a number of resonances in the PO collision complex. These resonances are the main driver for dissociative recombination, which is likely to be the main destroyer of ions such as PO^+ in low temperature plasmas such as the interstellar medium. It would be possible to extend the current study to provide the necessary inputs for studies of dissociative recombination as has been done for analogous NO^+ molecular ions (Rabadan and Tennyson 1997, Schneider *et al* 2000, Motapon *et al* 2006).

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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Supplementary data

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