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The radiative association of P and O atoms

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ABSTRACT

The formation of PO from the radiative association of phosphorus and oxygen atoms has been estimated by accurate quantum chemistry calculations. The radiative association of P and O atoms along the $B^2\Sigma^+$ potential energy curve is the most efficient way of producing PO in the $X^2\Pi$ ground state. For temperatures ranging between 300 and 14 000 K, the rate coefficients are found to vary from 1.61×10^{-24} to 1.99×10^{-18} cm^3s^{-1}, respectively. These values indicate that only a very small amount of PO molecules can be formed by radiative association in dense and hot gas close to the photosphere of evolved oxygen-rich stars and other hostile environments.

Key words: atomic data – atomic processes – molecular data – circumstellar matter – ISM: molecules.

1 INTRODUCTION

Phosphorus monoxide (PO) lines have been observed in the circumstellar envelopes of the star VY CMa (Tenenbaum, Woolf & Ziurys 2007; Tenenbaum et al. 2010; Kamiński et al. 2013a). VY CMa is an oxygen-rich (C/O abundance ratio < 1) red supergiant star with an effective temperature near 3200–3650 K (Massey, Levesque & Plez 2006; Wittkowski et al. 2012). Shock waves arising from pulsation of the star can levitate the stellar material, causing a large and variable mass-loss rate of 0.5×10^{-4}–3.0×10^{-3} $M_\odot$ yr^{-1} (Monnier, Tuthill & Lopez 1999; Wittkowski et al. 2012). This mass-loss rate produces an extended (1500–3000 $R_\odot$) outflowing circumstellar envelope. VY CMa is thought to have evolved from a massive star of ~ 25 $M_\odot$, then reduced to its present ~ 17 $M_\odot$ (Wittkowski et al. 2012). Due to its observed parameters, it is predicted to become a supernova at any time (Royer et al. 2010).

PO has also been found towards the circumstellar envelope of the asymptotic giant branch (AGB) oxygen star IK Tau (Sánches Contreras, Vellila Prieto & Cernicharo 2011; De Beck et al. 2013). On the other hand, the search for PO towards the oxygen-rich AGB star OH 231.8+4.2 has been unfruitful (Sánches Contreras et al 2011).

AGB stars represent a late stage of stellar evolution of low- and intermediate-mass stars, in the range 1.0–8.0 $M_\odot$, characterized by an effective temperature near 2000–3500 K (Herwig 2005; Iben & Renzini 1983). Because of instabilities in their interiors, AGB stars pulsate and can elevate material above the stellar surface, causing intense mass loss (Vassiliadis & Wood 1993). This high mass-loss rate (10^{-6}–10^{-4} $M_\odot$ yr^{-1}) progressively forms an extended (up to several au) outflowing envelope (Kwok 2000).

In our Galaxy, the initial element abundance of oxygen exceeds that of carbon and the stars are O-rich (Zhukovska, Gail & Trieloff 2008). Dredge-up of carbon, synthesized in the stellar interior, may turn a star with initial mass in the range $\sim$1.0–4.0 $M_\odot$ into a carbon-rich star (Herwig 2005), in which the C/O ratio exceeds unity. By contrast, in stars with initial masses in the range 4.0–8.0 $M_\odot$, carbon is converted into ^{14}N via the CN cycle, resulting in more oxygen than carbon in their atmospheres (Vassiliadis & Wood 1993; Herwig 2005).

Observations indicate that PO is formed in the inner regions of the O-rich shells of evolved stars (Tenenbaum et al. 2007; De Beck et al. 2013). Given the relatively dense and hot gas in the region, theoretical studies suggest that molecular compounds are formed in thermochemical equilibrium (TE: e.g. Tsuji 1973) and they are ejected as 'parent molecules' into the outer envelope, in which photochemistry creates other species (Willacy & Millar 1997; MacKay & Charnley 2001). The TE calculations of Tsuji (1973) predict that PS should be the major P-bearing molecule in the gas phase of an O-rich shell. However, only PO and PN have been observed in the inner region of the circumstellar envelopes of O-rich evolved stars (Tenenbaum et al. 2007, 2010; Milam et al. 2008; De Beck et al. 2013; Kamiński et al. 2013a). PS and PH_3 compounds have been sought in the wind of the O-rich star IK Tau at a comparable level, but have not been observed (De Beck et al. 2013). Both PO and PN disappear in the outer envelope, suggesting that they are converted to other species or condensed into dust grains (Tenenbaum et al. 2007; De Beck et al. 2013). Indeed, iron–nickel–phosphide compound was found in meteorites (Pasek & Lauretta 2005), the main solid-state carrier of phosphorus, which condenses at $\sim$1800 K (Lodders & Fegley 1999).

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The most recent TE models predict an abundance of PO close to those observed. On the other hand, the abundance of PN is about two orders of magnitude too low (Agúndez, Cernicharo & Guélin 2007; Milam et al. 2008). Another possible scenario for unexpected species production may be through shocks, triggered by the pulsation of the stars (e.g. Cherchneff 2012). Non-equilibrium chemistry triggered by shocks in the inner wind of C-rich stars could form PN very efficiently in post-shock gas (Cherchneff 2012), but PO was not included in this study. Following observations, PO appears to be the dominant carrier of phosphorus in the inner winds of O-rich evolved stars (Tenenbaum et al. 2007; De Beck et al. 2013). However, the chemical network involving phosphorus is poorly documented (Cherchneff 2012) and, within the set of all possible reactions for the formation of PO in photospheric gas, the rate coefficients for radiative association of P and O atoms should be known. Thus, we have investigated the formation of PO from the P(^{4}S) + O(^{3}P) reaction paths.

2 METHODS

2.1 Molecular data

The potential energy curves and transition moments needed in the radiative association calculus have been calculated by the multireference configuration interaction (MRCI) approach, based on complete active space self-consistent field (CASSCF) wavefunctions (Roos 1987), as implemented in the MOLPRO code (Werner et al. 2012). Full electron cc–pVQZ basis sets (Dunning 1989; Woon & Dunning 1993) were employed to describe the atomic species, augmented by three s (exp: 0.0384, 0.0158, 0.0065), three p (0.0292, 0.0110, 0.0042), three d (0.0656, 0.0262, 0.0104) and three f (0.1115, 0.0444, 0.0177) functions on the P atom only (Spielfiedel & Handy 1999). The CASSCF zeroth-order wavefunctions were generated including all phosphorus and oxygen valence electrons and orbitals in the active space (5–8σ, 2–3π valence orbitals), plus one extra σ and π orbital, resulting in a final (5–9σ, 2–4π) active space. The PO diatomic molecule belongs to the $C_{\infty v}$ Abelian point group but, for technical reasons, the highest point group available is the D_{2h}. To overcome this limitation, all calculations were carried out using the Abelian C_{2v} point-group symmetry (the z-axis being the internuclear axis), averaging simultaneously over the first three lowest-lying doublet electronic states belonging to the A_1 irreducible representation (IREP), the first three belonging to $B_{1,2}$ and the first two of the A_2 IREPs, as was done in another work (Singh et al. 1999). The quartet state was computed individually for each irreducible representation. Dynamic correlation effects were incorporated in the multireference configuration interaction with internal contraction level (ICMRCI: Werner & Knowles 1988; Knowles & Werner 1988), with the CASSCF wavefunctions described previously as zeroth-order wavefunctions. Potential energy functions were obtained by fitting cubic splines to the computed MRCI energies, which were used to compute vibrational wavefunctions and energies by numerical integration of the rovibrational Schrödinger equation with the program VIBROT (Karlström et al. 2003).

2.2 Radiative association

The rate coefficients at a given temperature T are estimated following the procedure used in previous works (e.g. Andreazza & de Almeida 2014), in which the cross-section for the process is determined in a semiclassical scheme (Bates 1951). This description of nuclear motion may be applied to collision of massive reactants (Zygelman & Dalgarno 1988), which form large dissociation energy products (Gustafsson 2013). In this approximation, the cross-section is given by

$$\sigma(E) = 4\pi P \left(\frac{\mu}{2E}\right)^{1/2} \int_0^\infty b\,\mathrm{d}b \int_{r_c}^\infty \frac{A(r)\,\mathrm{d}r}{\left[1 - \frac{V_{\Lambda^u S}(r)}{E} - \frac{b^2}{r^2}\right]^{1/2}}, \quad (1)$$

in which μ is the reduced mass, b is the impact parameter, E is the energy of the colliding particles, r_c is the distance of closest approach, P is the probability of approach along any particular molecular potential energy curve and $V_{\Lambda^u S}$ is the molecular potential energy curve through which the colliding particles unite. $A(r)$ is the transition probability for emission and is obtained by the expression

$$A(r) = 2.03 \times 10^{-6} \frac{(2 - \delta_{0,\Lambda^u+\Lambda^l})}{(2 - \delta_{0,\Lambda^u})} |\nu(r)|^3 |R_e(r)|^2 \ \mathrm{s}^{-1}, \quad (2)$$

in which $\nu(r)$ is the transition frequency in terms of wavenumbers (cm^{-1}) at internuclear distance r, $(2 - \delta_{0,\Lambda^u+\Lambda^l})/(2 - \delta_{0,\Lambda^u})$ is the degeneracy factor, $R_e(r)$ is the electronic dipole transition moment of electronic transition in atomic units and Λ^u and Λ^l are the components of electronic orbital angular momentum of the upper and lower electronic states, respectively, along the internuclear axis of the formed molecule.

The rate coefficient for the process at temperature T is obtained from an average of the cross-section over a Maxwell–Boltzmann distribution of kinetic energies, as

$$k(T) = \left(\frac{8}{\mu\pi}\right)^{1/2} \left(\frac{1}{k_B T}\right)^{3/2} \int_0^\infty E\,\sigma(E) \exp\left(-\frac{E}{k_B T}\right) \mathrm{d}E, \quad (3)$$

where k_B is the Boltzmann constant.

3 RESULTS AND DISCUSSION

The largest radiative association rate coefficients result when two atoms approach through an excited potential energy curve with potential minima lower than the dissociation limit and radiate via a strong dipole transition to the ground state (Herbst & Bates 1988). In a typical oxygen-rich envelope of an evolved star, with temperature near 2000–3500 K, only molecular states correlating with the ground-state asymptote need to be considered. In this way, the coupling of ground-state phosphorus (^{4}S) and oxygen (^{3}P) atoms can occurs through PO molecular electronic states Π and Σ^+, each of doublet, quartet and sextet multiplicities. The $1^4\Sigma^+$, $1^6\Pi$, $1^6\Sigma^+$, $X^2\Pi$, $B^2\Sigma^+$ and $a^4\Pi$ states have been characterized theoretically (Spielfiedel & Handy 1999; Liu et al. 2013; Izzaouihda et al. 2014). Of these, $X^2\Pi$, $B^2\Sigma^+$ and $a^4\Pi$ states have been identified spectroscopically (Huber & Herzberg 1979).

The radiative association of the P and O atoms, both in their ground states, can occur following approach along the $1^4\Sigma^+$, $1^6\Pi$, $1^6\Sigma^+$, $B^2\Sigma^+$ and $a^4\Pi$ states. The $1^4\Sigma^+$, $1^6\Pi$, $1^6\Sigma^+$ states are entirely repulsive (Liu et al. 2013; Izzaouihda et al. 2014). Because they make a negligible contribution to radiative association, transitions from a repulsive state are not considered here.

Attractive potential energy functions of relevant states correlating with the first dissociation asymptotes (P(^{4}S) + O(^{3}P)) and the corresponding transition moments as functions of the internuclear distance (r) are displayed in Figs 1 and 2, respectively. In the region $r \geq 2.2a_0$, the potential curves and dipole moments were obtained from *ab initio* calculations. In the short internuclear region ($r \leq 2.2a_0$), the potential curves and dipole moments were extrapolated

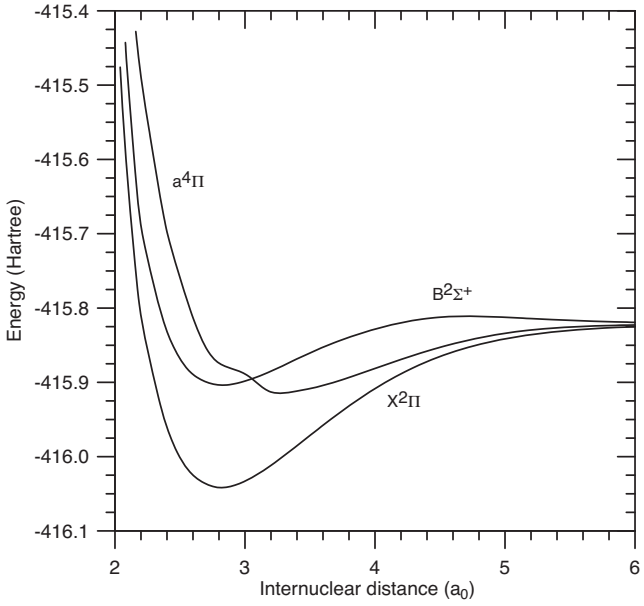

Figure 1. Potential energy curves for the doublet states of PO.

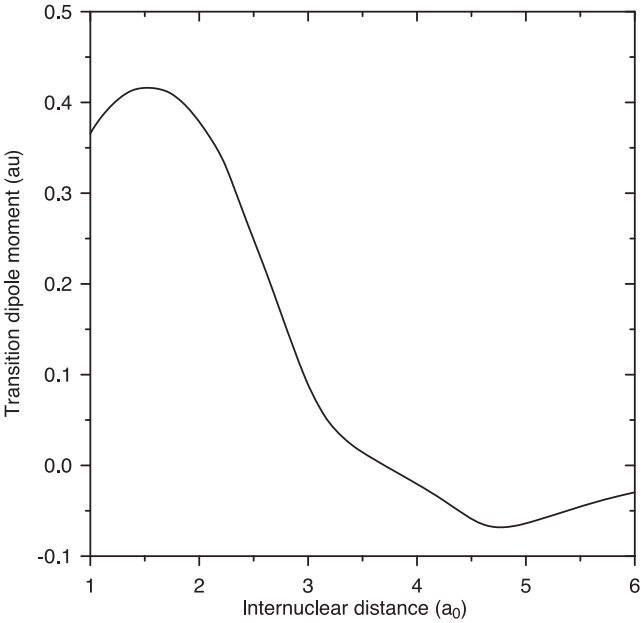

Figure 2. Electronic transition moment function between the doublet states of PO.

(Stancil et al. 1997) using a cubic spline and joined smoothly with the forms $V(r) = a\exp(-br) + c$ and $R_e(r) = ar^2 + br$, respectively. For the $X^2\Pi$ and $B^2\Sigma^+$ states, accurate experimental spectroscopic constants are available in the literature (Huber & Herzberg 1979). For the $a^4\Pi$ state, inaccurate experimental values can be found (Huber & Herzberg 1979; Grein & Kapur 1983). For a convenient comparison, the spectroscopic constants are given in Table 1 together with the experimental values and other theoretical results (Spielfiedel & Handy 1999; Liu et al. 2013; Izzaouihda et al. 2014), including the equilibrium distance (R_e), harmonic wavenumber (ω_e) and excitation energy (T_e). The present molecular constants are in good agreement with experimental measurements, to within 0.031 Å for R_e, 122 cm^{-1} for ω_e and 0.11 eV for T_e. For the $a^4\Pi$ state, the

Table 1. Molecular constants for the electronic states of PO.

		$X^2\Pi$	$a^4\Pi$	$B^2\Sigma^+$
R_e (Å)	This work	1.489	1.731	1.494
	Exp.[a, b]	1.476	(1.750)[f]	1.463
	MRCI+Q[c]	1.489	1.732	1.478
	MRCI+Q[d]	1.474	1.714	1.455
	MRCI[e]	1.482	1.713	1.463
ω_e (cm^{-1})	This work	1243	1156	1042
	Exp.[a, b]	1233		1164
	MRCI+Q[c]	1218	753	1129
	MRCI+Q[d]	1234	766	1186
	MRCI[e]	1215	771	1174
T_e (eV)	This work		3.43	3.75
	Exp.[a, b]		(3.00)	3.81
	MRCI+Q[c]		3.41	3.84
	MRCI+Q[d]		3.52	3.78
	MRCI[e]		3.43	3.85

Notes. [a] Huber & Herzberg (1979). [b]Grein & Kapur (1983). [c]Spielfiedel & Handy (1999) (MRCI+Q: MRCI methods plus the Dadidson correction (+Q)). [d]Liu et al. (2013). [e]Izzaouihda et al. (2014). [f]The results in brackets are not accurate.

Table 2. Radiative association rate coefficients of PO.

T (K)	k ($cm^3\ s^{-1}$)
300	1.61×10^{-24}
700	5.06×10^{-21}
1000	2.79×10^{-20}
1500	1.10×10^{-19}
2000	2.27×10^{-19}
2500	3.58×10^{-19}
3000	4.90×10^{-19}
3500	6.19×10^{-19}
4000	7.41×10^{-19}
4500	8.56×10^{-19}
5000	9.62×10^{-18}
6000	1.15×10^{-18}
7000	1.31×10^{-18}
8000	1.45×10^{-18}
10 000	1.68×10^{-18}
12 000	1.85×10^{-18}
14 000	1.99×10^{-18}

values of R_e, ω_e and T_e are also in good agreement with those calculated previously. To the best of our knowledge, no theoretical transition moments as functions of the internuclear distance have been published in the literature.

Radiative association of ground-state phosphorus and oxygen atoms can occur following approach along the $B^2\Sigma^+$ state, which radiates to the ground $X^2\Pi$ state of PO. The probability of approach along the $B^2\Sigma^+$ state is 1/18.

The rate coefficients for approach along the $B^2\Sigma^+$ state are listed in Table 2. They are found to vary from 1.61×10^{-24} to 1.99×10^{-18} $cm^3\ s^{-1}$ for temperatures ranging from 300–14 000 K, respectively, and can be approximated (within 7 per cent) as

$$k(T) = 8.29 \times 10^{-18} \left(\frac{T}{300}\right)^{-0.917} \exp\left(\frac{-4636}{T}\right)\ cm^3\ s^{-1} \quad (4)$$

for temperatures between 300 and 1000 K and

$$k(T) = 1.99 \times 10^{-18} \left(\frac{T}{300}\right)^{0.065} \exp\left(\frac{-4462}{T}\right) \text{ cm}^3 \text{ s}^{-1} \qquad (5)$$

for temperatures higher than 1000 K.

Because we do not take into account the fine structure of the phosphorus atom (∼227 cm^{-1}), our predicted rate coefficients are uncertain at temperatures lower than about 327 K. Moreover, the $B^2\Sigma^+$ state has a barrier against dissociation into $P(^4S) + O(^3P)$. This has already been seen in the theoretical works of Liu et al. (2013) and Izzaouihda et al. (2014). Due to the potential barrier, the rate coefficients decrease rapidly at low temperatures. However, the height of the barrier is about 2416.49 cm^{-1} at $4.8a_0$, which is about 508.66 cm^{-1} lower than the value reported by Liu et al. (2013). Also, the barrier in our PO $B^2\Sigma^+$ potential appears to be significantly lower than the one shown in fig. 1 of Izzaouihda et al. (2014). The uncertainty in the barrier height results in a significant uncertainty in the rate coefficients at low temperatures. Other sources of error at low temperatures are quantum mechanical effects such as tunnelling and shape resonance (Bain & Bardsley 1972; Smith 1989; Gustafsson 2013). At 300 K, quantum mechanical calculations (Antipov et al. 2009; Franz, Gustafsson & Nyman 2011) show that the classical calculations (Dalgarno, Du & You 1990; Singh et al. 1999; Singh & Andreazza 2000) underestimate the rate coefficients by about 25 per cent and one order of magnitude for CN (Singh & Andreazza 2000) and CO (Dalgarno et al. 1990; Singh et al. 1999) formation, respectively. At temperatures higher than 1000 K, the quantum mechanical (Antipov et al. 2009; Gustafsson 2013) and semiclassical (Dalgarno et al. 1990; Singh et al. 1999; Singh & Andreazza 2000) rate coefficients are in good agreement. In these studies, CN and CO formation was assumed to occur mainly through the $A^2\Pi$ and $A^1\Pi$ states, respectively. The former potential curve has no barrier, while the latter shows a potential hump. In semiclassical studies, Dalgarno et al. (1990) and Singh et al. (1999) used the same set of potentials for the $A^1\Pi$ and $X^1\Sigma^+$ states of CO and different transition dipole moment functions. The rate coefficients obtained by these authors are in agreemnet with each other. However, in quantum mechanical calculations, Franz et al. (2011) used a different set of potentials with a low barrier height for the $A^1\Pi$ state of CO. For CO, the resonance contribution to the rate coefficients arises from quantum mechanical tunnelling through the barrier (Franz et al. 2011). At low temperatures, both quantum mechanical and semiclassical theories depend strongly on barrier height. As previously mentioned, the uncertainty in barrier height results in a significant uncertainty in the rate coefficients at low temperatures. Considering all these effects, mainly the uncertainty in barrier height, it is likely that the values in Table 1 have a discrepancy of about two orders of magnitude at 300 K. For temperatures higher than 1000 K, an error of one order of magnitude is more appropriate for the estimated rate coefficients in Table 2.

For 1500 and 3500 K (the range of temperature where formation of PO in the circumstellar envelope is relevant), our calculated radiative association rate coefficients for P and O atoms are 1.10×10^{-19} and 6.19×10^{-19} $cm^3\ s^{-1}$, respectively. The corresponding rate coefficients for SiO are 5.63×10^{-17} and 7.11×10^{-17} $cm^3\ s^{-1}$ (Andreazza, Singh & Sanzovo 1995), those for TiO are 7.46×10^{-17} and 8.84×10^{-17} $cm^3\ s^{-1}$ (Andreazza et al. 2012) and those for SiS are 1.52×10^{-16} and 2.15×10^{-16} $cm^3\ s^{-1}$ (Andreazza & Marinho 2007). These values show that Si+O, Ti+O and Si+S reactions are two to three orders of magnitude higher than the corresponding P+O reaction. Hence, the radiative association of P and O atoms to form the PO radical is slow, as expected for the formation of a massive diatomic molecule, involving an attractive potential along with the colliding atoms which can penetrate to small distance.

4 CONCLUSIONS

The rate coefficients for radiative association of P and O atoms to form the PO molecule are estimated. The molecule-forming transitions were assumed to occur dominantly through the $B^2\Sigma^+$ state, followed by radiative transition to the $X^2\Pi$ state. They are found to vary from 1.61×10^{-24} to 1.99×10^{-18} $cm^3\ s^{-1}$ for temperatures ranging from 300–14 000 K, respectively.

The rate coefficients for the radiative association of PO are of the order of 1.10×10^{-19} to 6.19×10^{-19} $cm^3\ s^{-1}$ for temperatures of 1500–3500 K. These values are low, as expected for the formation of a massive diatomic molecule through the radiative association process, involving an excited state with potential minima lower than the dissociation limit of the ground state. These results also indicate that only a very small amount of PO can be formed by radiative association in the inner envelopes of oxygen-rich stars and other hostile environments.

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