Structural, spectroscopic and energetic parameters of P-bearing species having astrophysical importance

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Kevin Gooniah1,2, Hanshika Jhurree2, Lydia Rhyman2, Ibrahim A. Alswaidan1, Hoong-Kun Fun1,4, Radhakhrishna Somanah1 and Ponnadurai Ramasami2,3*

Abstract: Molecular parameters such as equilibrium structure, dipole moment, rotational constant, harmonic frequency, IR intensity, adiabatic electron affinity, atomisation energy and ionisation potential of some P-bearing molecules PS, PO and HC₃P in their neutral, cationic and anionic forms were investigated using the popular B3LYP hybrid density functional with four basis sets 6-311++G(2df,2pd), 6-311++G(3df,3pd), cc-pVTZ and aug-cc-pVTZ. The computed data conform well to those existing in the literature. Therefore, the predicted data for those molecules or ions which are not available in the literature should be reliable.

1. Introduction

Agúndez, Cernicharo, and Guélin (2007) detected phosphaethyne (HCP) in the AGB star envelope IRC +10216. According to chemical models performed by Agúndez et al. (2007), other P-bearing molecules that are likely to be detected are phosphorus monosulphide (PS) and phosphorus monoxide (PO) in O-rich circumstellar envelopes and phosphabutadiyne (HC₃P) in C-rich circumstellar envelopes. The identification of HC₃P is highly probable due to the reaction between carbon monophosphide (CP) and acetylene (C₂H₂), CP + C₂H₂ → HC₃P + H, studied theoretically by Yu, Zhao, Kan, and Fu (2006) using B3LYP and QCSID(T) methods.
Interstellar grain mass is mostly formed by accretion—a process directly related to the depletion of elements. Phosphorus is generally believed to be highly depleted in dense molecular clouds. As pointed out by Agúndez et al. (2007), phosphorus should be present in the hot stellar atmospheres of late-stage stars and thermochemical equilibrium calculations suggest that it is locked into PS and PO (O-rich envelopes) or HCP (C-rich envelopes). When a cold envelope is formed through the expansion of the atmospheric gas, most of the heavy elements condense on dust grains. The observation and study of the P-bearing molecules are thereby important for understanding the chemistry of grains in interstellar/circumstellar medium.

Experimental work on the equilibrium structures of PO and PS molecules involves spectroscopic investigation by Huber and Herzberg (1979). The electron affinity (EA) of PO was studied by Brinkmann, Tschumper, and Schaefer (1999) where they employed six functionals. They also rendered values for the optimised structures and harmonic frequencies of PO and its anion PO−. Zittel and Lineberger (1976) utilised a fixed-frequency laser photoelectron spectroscopy to study beams of PO− produced from phosphine burned with N2O in a low-pressure discharge source. They obtained an EA of 1.092 ± 0.010 eV for PO molecule. Dyke, Morris, and Ridha (1982) studied the ground state of PO+ by means of a vacuum ultraviolet photoelectron spectroscopy and the adiabatic ionisation potential (IP) of PO was measured as 8.39 ± 0.01 eV. The G2 value determined by Curtiss, Raghavachari, Trucks, and Pople (1991) for the atomisation energy (AE) of PO is 98.9 kcal/mol. Metropoulos, Papakondylis, and Movridis (2003) computed the accurate potential energy curves of the ground states of the PO, PO+ and PO− species using multireference method. Müller and Woon (2013) calculated the dipole moments for silicon and phosphorus compounds of astrophysical interest.

Botschwina, Oswald, Linnartz, and Verdes (2000) reported the equilibrium geometry, harmonic vibrational wavenumbers, vibration–rotation coupling constant and l-type doubling constants of HC3P molecule using CCSD(T) method. The only experimental investigation of HC3P is the study of the microwave spectrum by Kroto, Nixon, and Ohno (1981), from which rotational, quartic centrifugal distortions and l-type doubling constants were determined. No experimental and theoretical findings are available for the anion and cation of HC3P molecule.

This theoretical research targets some identified and potential (P-bearing) interstellar molecules using the B3LYP functional and four basis sets. The objectives of this work were: (1) to assess the performance of the functional and the basis sets to calculate structural, spectroscopic and energetic parameters and (2) to ascertain the computed parameters for those not yet available in the literature.

2. Methodology
The hybrid density functional B3LYP was employed to provide insight into the molecular properties of the potential P-bearing interstellar molecules. Computations were performed using four different basis sets 6-311++G(2df,2pd), 6-311++G(3df,3pd), cc-pVTZ and aug-cc-pVTZ (Clark, Chandrasekhar, Spitznagel, & Schleyer, 1983; Dunning, 1989; Frisch, Pople, & Binkley, 1984; Gill, Johnson, Pople, & Frisch, 1992; Kendall, Dunning, & Harrison, 1992; Woon & Dunning, 1993). For each basis set, the molecular structures were optimised under tight convergence criteria and frequency computations were carried out to verify the nature of the stationary points. Similar procedures were applied to the anion and cation of each species. All computations were performed using a suite of Gaussian 03W programs (Frisch et al., 2003).

The adiabatic EA, $EA = E(\text{optimised neutral}) - E(\text{optimised anion})$, of each molecule was computed as the difference between the total energy of the optimised neutral molecule and the total energy of the corresponding optimised anion.

The AE was calculated as the energy difference between the optimised neutral molecule and its corresponding constituent atoms. Adiabatic IP is the energy necessary to remove an electron from the outermost filled molecular orbital of the ground state.
The adiabatic IP, \( \text{IP} = E(\text{optimised neutral}) - E(\text{optimised cation}) \), was computed as the difference between the total energy of the optimised neutral molecule and the total energy of the corresponding optimised cation.

3. Results and discussion

3.1. Equilibrium geometries of potential P-bearing astromolecules

The computed equilibrium bond lengths of the two P-bearing diatomic molecules with their anions and cations are shown in Table 1 along with empirical and earlier theoretical data. The 6-311++G(3df,3pd) basis set produces lower values compared to the other three basis sets. The cc-pVTZ and aug-cc-pVTZ basis sets rendered similar values for the studied phosphorus-bearing species except for PS\(^{-}\) and PO\(^{-}\). For PS molecule, the predicted 6-311++G(3df,3pd) value is quite close to the experimental value of Huber and Herzberg (1979) while the 6-311++G(2df,2pd) value of PS deviates by about 0.006 Å. The deviation of the remaining computed values using the other three basis sets is 0.011 Å. Good agreement is observed between the computed 6-311++G(3df,3pd) value of PO and the experimental value (Huber & Herzberg, 1979) with deviation of 0.002 Å. The cc-pVTZ and aug-cc-pVTZ values of PO are nevertheless in better agreement with the theoretical result of Brinkmann et al. (1999). For PO\(^{-}\), the aug-cc-pVTZ basis set produces a value that remarkably concurs with the experimental result, and hence predicts a much better value than that computed by Brinkmann et al. (1999). Deviation is comparatively significant (about 0.02 Å) for PO\(^{-}\) using the cc-pVTZ basis set with reference to the experimental value. It is noted that cc-pVTZ value of PO\(^{-}\) differs quite considerably to the values obtained from the other three basis sets.

Table 2 illustrates the optimised structural parameters of HC\(_3\)P, HC\(_3\)P\(^{-}\) and HC\(_3\)P\(^{+}\). Contrary to HC\(_3\)P and HC\(_3\)P\(^{+}\), a non-linear minima was located for HC\(_3\)P\(^{-}\) (Figure 1) using the four basis sets.

The computed structural parameters of HC\(_3\)P agree quite well with the CCSD(T)/cc-pVTZ result of Botschwina et al. (2000). The 6-311++G(2df,2pd) and aug-cc-pVTZ basis sets produce values of R(HC\(_1\)) that are identical to the corresponding estimated value of Botschwina et al. (2000) while the other two basis sets underestimate by only 0.001 Å. For the four basis sets, the calculated values of R(C\(_1\)C\(_2\)) are similar and deviate from the corresponding CCSD(T) result by 0.003 Å. A similar situation is observed for the predicted values of R(C\(_1\)C\(_2\)) but with a deviation of 0.012 Å with its corresponding CCSD(T) result. For the structural parameter R(C\(_1\)P), the 6-311++G(2df,2pd) value is in better agreement with the CCSD(T) result than the computed values at the other three basis sets. No experimental and earlier theoretical findings are available for HC\(_3\)P\(^{-}\) and HC\(_3\)P\(^{+}\) ions. The optimised geometries of the anionic and cationic species are hence reported for the first time. The computed structural parameters of HC\(_3\)P\(^{-}\) do not differ significantly from each other using the four basis sets. For the bond angles \( \theta(\text{HC}_1\text{C}_2) \) and \( \theta(\text{C}_1\text{C}_2\text{P}) \), the predicted cc-pVTZ values are however, found to be lower than the values using the other three basis sets.

3.2. Dipole moments of potential P-bearing astromolecules

Table 3 displays the results of the computed dipole moments of the P-bearing species. Experimental and earlier estimated values are only available for HC\(_3\)P molecule. The aug-cc-pVTZ value is closer with the CCSD(T)/cc-pVTZ value of Botschwina et al. (2000). Nevertheless, the aug-cc-pVTZ value differs by 0.125 D from the dipole moment obtained by Kroto et al. (1981). The 6-311++G(3df,3pd) produces a value that deviates less from the experimental dipole moment of HC\(_3\)P compared to the predictions of the other three basis sets. For PS\(^{-}\) molecule, the cc-pVTZ value is particularly lower than the other computed dipole moments. Also, it is noted that the calculated dipole moments of PO\(^{-}\) molecule increase quite significantly with the enhancement of the basis set from 6-311++G(2df,2pd) to aug-cc-pVTZ.

3.3. Rotational constants of potential P-bearing astromolecules

The computed rotational constants of the P-bearing species are compiled in Table 4. For PS, the 6-311++G(3df,3pd) basis set renders values that conform very well with the observed value (Huber & Herzberg, 1979) with a deviation of only 0.002 GHz. For PO molecule, the 6-311++G(3df,3pd) value deviates from the corresponding empirical value (Huber & Herzberg, 1979) by 0.047 GHz while the
Table 1. Bond lengths (Å) of PS, PO, and their anions and cations

| Molecules/ions | Basis sets          | Other values          |
|---------------|---------------------|-----------------------|
|               | 6-311++G(2df,2pd)   | 6-311++G(3df,3pd)     | cc-pVTZ                | aug-cc-pVTZ | Theoretical | Experimental |
| PS            | 1.906               | 1.902                 | 1.911                  | 1.911       | -           | 1.90a        |
| PS−           | 2.005               | 2.000                 | 2.021                  | 2.009       | -           | -            |
| PS+           | 1.829               | 1.825                 | 1.833                  | 1.833       | -           | -            |
| PO            | 1.481               | 1.478                 | 1.487                  | 1.487       | 1.493b      | 1.476a       |
| PO−           | 1.537               | 1.533                 | 1.560                  | 1.541       | 1.548b      | 1.540c       |
| PO+           | 1.425               | 1.422                 | 1.431                  | 1.431       | -           | -            |

*aHuber and Herzberg (1979).  
bBrinkmann et al. (1999).  
cValue quoted in Brinkmann et al. (1999).

Table 2. Equilibrium geometries of HC₃P, HC₃P− and HC₃P+

| Molecules/ions | Basis sets          | Other values          |
|---------------|---------------------|-----------------------|
|               | 6-311++G(2df,2pd)   | 6-311++G(3df,3pd)     | cc-pVTZ                | aug-cc-pVTZ | Theoretical |
| HC₃P          | R(HC₁) 1.062        | R(HC₁) 1.061          | 1.061                  | 1.062       | 1.062a      |
|               | R(C₁C₂) 1.210       | R(C₁C₂) 1.210         | 1.210                  | 1.210       | 1.213b      |
|               | R(C₂C₃) 1.355       | R(C₂C₃) 1.355         | 1.355                  | 1.355       | 1.367b      |
|               | R(C₃P) 1.550        | R(C₃P) 1.549          | 1.554                  | 1.554       | 1.551b      |
| HC₃P−         | R(HC₁) 1.082        | R(HC₁) 1.082          | 1.085                  | 1.082       | -           |
|               | R(C₁C₂) 1.268       | R(C₁C₂) 1.268         | 1.271                  | 1.268       | -           |
|               | R(C₂C₃) 1.317       | R(C₂C₃) 1.318         | 1.316                  | 1.317       | -           |
|               | R(C₃P) 1.609        | R(C₃P) 1.607          | 1.614                  | 1.613       | -           |
|               | θ(HC₁C₂C₃) 132.1     | θ(HC₁C₂C₃) 132.2      | 130.1                  | 132.1       | -           |
|               | θ(C₁C₂C₃) 172.7      | θ(C₁C₂C₃) 172.7       | 172.6                  | 172.6       | -           |
|               | θ(C₃P) 178.8        | θ(C₃P) 178.8          | 177.7                  | 178.7       | -           |
| HC₃P+         | R(HC₁) 1.071        | R(HC₁) 1.071          | 1.071                  | 1.071       | -           |
|               | R(C₁C₂) 1.230       | R(C₁C₂) 1.230         | 1.230                  | 1.230       | -           |
|               | R(C₂C₃) 1.319       | R(C₂C₃) 1.320         | 1.320                  | 1.319       | -           |
|               | R(C₃P) 1.588        | R(C₃P) 1.587          | 1.592                  | 1.592       | -           |

Notes: Bond lengths are in angstroms (Å) and bond angles θ in degrees (°).  
bBotschwina et al. (2000).
deviations for the other calculated values are more significant. The computed values of HC$_3$P deviate with less than 0.03 GHz from the experimental value (Kroto et al., 1981) as well as the estimated value of Botschwina et al. (2000). The cc-pVTZ value of HC$_3$P$^-$ is quite low compared to the predicted values using the other three basis sets. For the remaining molecules, no experimental and earlier theoretical data are available for comparison.

3.4. Harmonic frequencies and IR intensities of potential P-bearing astromolecules
Table 5 shows the calculated harmonic frequencies and IR intensities (in parenthesis) of PS, PO, and their respective anions and cations. The cc-pVTZ and aug-cc-pVTZ values of PS concord very well with the experimental value (Huber & Herzberg, 1979) compared the other computed values using the other two basis sets. The calculated harmonic frequencies of PO deviate from the experimental value (Huber & Herzberg, 1979) by less than 26 cm$^{-1}$. The aug-cc-pVTZ value of PO is nevertheless closer to the theoretical value of Brinkmann et al. (1999) than the experimental result. For PO$^-$, all the computed harmonic frequencies fall within the error bar of the experimental value. The trend in the computed values of all molecules is their decrease from 6-311++G(3df,3pd) to aug-cc-pVTZ.

The calculated harmonic frequencies of HC$_3$P are given in Table 6 with the IR intensities in parenthesis. The computations of the harmonic frequencies of HC$_3$P agree very well with the coupled cluster calculation of Botschwina et al. (2000). Good agreement is observed for the calculated bending frequencies $\nu_5$ with the experimental value, nearly all the estimated values fall within the experimental error bar. It is to be noted that the computed bending frequencies $\nu_5$ concur well with the experimental result.

For HC$_3$P$^-$ and HC$_3$P$^+$, the computed harmonic frequencies together with the IR intensities (in parenthesis) are presented in Tables 7 and 8. There are no experimental and earlier theoretical data available for comparison. The B3LYP approach using each of the four basis sets, all fail to produce degenerate frequencies for the bending modes for HC$_3$P$^+$.

3.5. Molecular energetics of potential P-bearing astromolecules
The electron affinities, atomisation energies and IPs of the P-bearing molecules are shown in Table 9. For PS molecule, the calculated atomisation energies are quite in good agreement with theoretical value (Curtiss et al., 1991) while the computed IPs are found to be smaller than the corresponding experimental value (Drowart, Myers, Szwarc, Vander Auwera-Mahieu, & Uy, 1973) by about 10%. For PO molecule, the aug-cc-pVTZ value of the EA is quite comparable to the estimated value of Brinkmann et al. (1999) but large deviations are however noticed for all its computed electron affinities from the experimental.

Table 3. Dipole moments (Debye) of the P-bearing molecules

| Molecules/ions | Basis sets | Other values |
|----------------|------------|--------------|
|                | 6-311++G(2df,2pd) | 6-311++G(3df,3pd) | cc-pVTZ | aug-cc-pVTZ | Theoretical | Experimental |
| PS             | 0.694       | 0.636        | 0.713   | 0.673       | –           | –           |
| PO             | 2.132       | 2.043        | 2.054   | 2.046       | –           | –           |
| PO$^-$         | 0.236       | 0.359        | 0.416   | 0.625       | –           | –           |
| PO$^+$         | 3.497       | 3.469        | 3.439   | 3.446       | –           | –           |
| HC$_3$P        | 0.826       | 0.814        | 0.890   | 0.870       | 0.849$^a$   | 0.745 ± 0.005$^a$ |
| HC$_3$P$^-$    | 1.222       | 1.188        | 1.305   | 1.171       | –           | –           |
| HC$_3$P$^+$    | 1.514       | 1.526        | 1.579   | 1.568       | –           | –           |

$^a$Botschwina et al. (2000).
$^b$Kroto et al. (1981).
Table 4. Rotational constants (GHz) of the P-bearing molecules

| Molecules/ions | Basis sets | Other values |
|----------------|------------|--------------|
|                | 6-311++G(2df,2pd) | 6-311++G(3df,3pd) | cc-pVTZ | aug-cc-pVTZ | Theoretical | Experimental |
| PS             | 8.839      | 8.881        | 8.792  | 8.797       | –           | 8.883b      |
| PS−            | 7.988      | 8.034        | 7.866  | 7.956       | –           | –           |
| PS+            | 9.604      | 9.642        | 9.557  | 9.558       | –           | –           |
| PO             | 21.853     | 21.948       | 21.667 | 21.672      | –           | 21.995b     |
| PO−            | 20.283     | 20.376       | 19.679 | 20.180      | –           | –           |
| PO+            | 23.593     | 23.681       | 23.408 | 23.397      | –           | –           |
| HC$_3$P        | 2.680      | 2.682        | 2.675  | 2.676       | 2.658a      | 2.656b      |
| HC$_3$P−       | A          | 968.806      | 971.486| 900.193     | 968.351     | –           | –           |
|                | B          | 2.628        | 2.630  | 2.622       | 2.623       | –           | –           |
|                | C          | 2.621        | 2.623  | 2.614       | 2.616       | –           | –           |

*Botschwina et al. (2000).  
*Kroto et al. (1981).

Table 5. Harmonic frequencies (cm$^{-1}$) and IR intensities (km/mol) of PS, PO, and their anions and cations

| Molecules/ions | Vibrational system | Basis sets | Other values |
|----------------|--------------------|------------|--------------|
|                |                    | 6-311++G(2df,2pd) | 6-311++G(3df,3pd) | cc-pVTZ | aug-cc-pVTZ | Theoretical | Experimental |
| PS             | Σ$^+$             | 745 (21.1)   | 747 (20.2)  | 741 (18.7) | 740 (20.2) | –           | 739a        |
| PS−            | Σ$^+$             | 870 (15.1)   | 872 (14.9)  | 865 (14.9) | 864 (14.8) | –           | –           |
| PO             | Σ$^+$             | 1255 (58.0)  | 1258 (57.5) | 1253 (41.9) | 1249 (57.5) | 1241a       | 1233s       |
| PO−            | Σ$^+$             | 1048 (156.5) | 1052 (146.5) | 1026 (56.9) | 1047 (171.1) | 1036a       | 1000 ± 70c  |

*Huber and Herzberg (1979).  
*Brinkmann et al. (1999).  
*Value quoted in Brinkmann et al. (1999).

Table 6. Harmonic frequencies (cm$^{-1}$) and IR intensities (km/mol) of HC$_3$P

| No. | Vibrational system | Basis sets | Other values |
|-----|--------------------|------------|--------------|
|     |                    | 6-311++G(2df,2pd) | 6-311++G(3df,3pd) | cc-pVTZ | aug-cc-pVTZ | Theoretical | Experimental |
| $v_1$ | Σ$^+$         | 3463 (103.2) | 3466 (102.6) | 3466 (101.9) | 3463 (99.4) | 3455        | –           |
| $v_2$ | Σ$^+$         | 2163 (9.2)   | 2163 (8.8)   | 2166 (11.9)  | 2163 (8.7)  | 2108        | –           |
| $v_3$ | Σ$^+$         | 1586 (37.8)  | 1587 (37.4)  | 1585 (33.3)  | 1583 (35.7) | 1536        | –           |
| $v_4$ | Σ$^+$         | 710 (0.1)    | 710 (0.1)    | 709 (0.1)    | 709 (0.2)   | 682         | –           |
| $v_5^*$ | Π               | 649 (44.9)   | 665 (41.8)   | 646 (43.3)   | 648 (40.3)  | 627         | 587 ± 77    |
| $v_6^*$ | Π               | 523 (0.9)    | 534 (0.03)   | 518 (1.0)    | 517 (0.7)   | 481         | 412 ± 54    |
| $v_7^*$ | Π               | 207 (0.9)    | 206 (8.1)    | 205 (6.5)    | 205 (8.0)   | 196         | 206 ± 27    |

*Doubly degenerate modes.  
*Botschwina et al. (2000).  
*Value quoted in Botschwina et al. (2000).
Table 7. Harmonic frequencies (cm\(^{-1}\)) and IR intensities (km/mol) of HC\(_3\)P\(^-\)

| No. | Vibrational system | Basis sets | 6-311++G(2df,2pd) | 6-311++G(3df,3pd) | cc-pVTZ | aug-cc-pVTZ |
|-----|--------------------|------------|------------------|------------------|---------|------------|
| \(\nu_1\) | \(a^\prime\) | 3153 (120.1) | 3155 (109.7) | 3116 (125.9) | 3149 (105.6) |
| \(\nu_2\) | \(a^\prime\) | 1947 (78.2) | 1948 (87.4) | 1955 (34.6) | 1947 (87.7) |
| \(\nu_3\) | \(a^\prime\) | 1462 (127.6) | 1462 (144.2) | 1457 (128.5) | 1459 (131.0) |
| \(\nu_4\) | \(a^\prime\) | 694 (116.3) | 695 (120.1) | 710 (231.0) | 690 (111.5) |
| \(\nu_5\) | \(a^\prime\) | 641 (327.8) | 642 (333.7) | 659 (161.0) | 638 (352.1) |
| \(\nu_6\) | \(a^\prime\) | 447 (27.9) | 444 (28.5) | 447 (31.1) | 439 (27.2) |
| \(\nu_7\) | \(a^\prime\) | 201 (4.8) | 194 (3.3) | 203 (2.4) | 194 (2.9) |
| \(\nu_8\) | \(a^\prime\) | 553 (0.5) | 550 (0.7) | 566 (1.1) | 544 (1.0) |
| \(\nu_9\) | \(a^\prime\) | 214 (0.5) | 211 (0.6) | 219 (0.2) | 211 (0.8) |

Table 8. Harmonic frequencies (cm\(^{-1}\)) and IR intensities (km/mol) of HC\(_3\)P\(^+\)

| No. | Vibrational system | Basis sets | 6-311++G(2df,2pd) | 6-311++G(3df,3pd) | cc-pVTZ | aug-cc-pVTZ |
|-----|--------------------|------------|------------------|------------------|---------|------------|
| \(\nu_1\) | \(\Sigma^+\) | 3375 (196.5) | 3378 (194.9) | 3375 (196.7) | 3374 (194.6) |
| \(\nu_2\) | \(\Sigma^+\) | 2112 (175.4) | 2113 (174.7) | 2112 (180.6) | 2111 (178.6) |
| \(\nu_3\) | \(\Sigma^+\) | 1509 (34.6) | 1510 (35.3) | 1506 (33.7) | 1506 (33.7) |
| \(\nu_4\) | \(\Sigma^+\) | 700 (2.4) | 700 (2.4) | 697 (2.4) | 698 (2.5) |
| \(\nu_5\) | \(\Pi\) | 771 (16.0) | 786 (15.2) | 772 (16.3) | 770 (15.2) |
| \(\nu_6\) | \(\Pi\) | 648 (43.4) | 664 (42.1) | 649 (43.7) | 648 (41.1) |
| \(\nu_7\) | \(\Pi\) | 504 (0.7) | 519 (0.0) | 495 (0.8) | 496 (0.6) |
| \(\nu_8\) | \(\Pi\) | 462 (1.2) | 468 (1.7) | 452 (1.2) | 452 (1.4) |
| \(\nu_9\) | \(\Pi\) | 193 (12.3) | 192 (12.1) | 191 (12.0) | 191 (11.7) |
| \(\nu_{10}\) | \(\Pi\) | 179 (8.6) | 176 (8.1) | 176 (8.5) | 176 (8.1) |

Table 9. Electron affinities (EA), atomisation energies (AE) and ionisation potentials (IP) in kcal/mol of the P-bearing molecules

| Molecules | Basis sets | 6-311++G(2df,2pd) | 6-311++G(3df,3pd) | cc-pVTZ | aug-cc-pVTZ | Other values | Theoretical | Experimental |
|-----------|------------|------------------|------------------|---------|------------|--------------|-------------|-------------|
| PS        | EA         | 19.0             | 18.7             | 12.4    | 19.7       | -            | -           | -           |
|           | AE         | 103.9            | 104.8            | 102.2   | 102.3      | 98.9\(^a\)  | 140 ± 25\(^a\) |
|           | IP         | 185.6            | 185.5            | 185.9   | 186.3      | -            | 207.5\(^a\) |
| PO        | EA         | 7.5              | 7.3              | -5.1    | 9.3        | 9.92\(^a\)  | 25.18 ± 0.23\(^a\) |
|           | AE         | 143.2            | 144.8            | 140.5   | 141.1      | 139.6\(^a\) | 141.8\(^a\) |
|           | IP         | 197.7            | 197.5            | 196.5   | 198.3      | -            | 193.48 ± 0.23\(^a\) |
| HC\(_3\)P | EA         | 15.8             | 15.8             | 12.0    | 16.2       | -            | -           | -           |
|           | AE         | 546.9            | 548.0            | 544.6   | 544.2      | -            | -           | -           |
|           | IP         | 218.1            | 218.2            | 217.8   | 218.0      | -            | -           | -           |

\(^a\)Curtiss et al. (1991).
\(^a\)Values quoted in Curtiss et al. (1991).
\(^a\)Drowart et al. (1973).
\(^a\)Brinkmann et al. (1999).
\(^a\)Zittel and Lineberger (1976).
\(^a\)Dyke et al. (1982).
result (Zittel & Lineberger, 1976). Good agreements are also observed for the predicted cc-pVTZ AE of PO with the G2 result of Curtiss et al. (1991) and for the aug-cc-pVTZ AE of PO with the corresponding observed value. In general, all the computed cc-pVTZ electron affinities are comparatively smaller than the electron affinities predicted at the other three basis sets. No experimental and earlier theoretical data are available for comparison with the computed EA, AE and IP of HC₃P.

4. Conclusions
The computed parameters agree quite well with structural information from experimental and earlier theoretical data wherever available. For molecules or ions not previously studied, the computed data should be reliable. All the four basis sets predict a non-linear minimum configuration for HC₃P⁻. For P-bearing molecules with exception to PS⁻, PO⁻, HC₃P and HC₃P⁺, the computed values decreases in general from 6-311++G(2df,2pd) to the aug-cc-pVTZ. The estimated rotational constants for P-bearing molecules decrease from 6-311++G(3df,3pd) to aug-cc-pVTZ. The estimated rotational constants for P-bearing species having astrophysical importance, Kevin Gooniah, Hanshika Jhurree, Lydia Rhyman, Ibrahim A. Alswaidan, Hoong-Kun Fun, Radhakhrishna Somanah and Ponnadurai Ramasami.

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Author details
Kevin Gooniah²
E-mail: vcccmru@gmail.com
Hanshika Jhurree²
E-mail: hanshika010@gmail.com
Lydia Rhyman²
E-mail: lyd.rhyman@gmail.com
Ibrahim A. Alswaidan¹
E-mail: aliiswaidan@ksu.edu.sa
Hoong-Kun Fun³⁴
E-mail: hfun@ksu.edu.sa
Radhakhrishna Somanah¹
E-mail: dinesh@uom.ac.mmu
Ponnadurai Ramasami³⁴
E-mail: ramchem@kninet.mu

¹ Department of Physics, University of Mauritius, RÉduit 80837, Mauritius.
² Computational Chemistry Group, Department of Chemistry, University of Mauritius, RÉduit 80837, Mauritius.
³ Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia.
⁴ X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia (USM), Penang 11800, Malaysia.

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References
Agúndez, M., Cernicharo, J., & Guélin, M. (2007). Discovery of phosphaethyne (HCP) in space: Phosphorus chemistry in circumstellar envelopes. The Astrophysical Journal, 662, L91–L94. Retrieved from http://iopscience.iop.org/1538-4357/662/2/L91
http://dx.doi.org/10.1086/519561
Botschewina, P., Oswald, R., Linnartz, H., & Verdes, D. (2000). The σ, π, and π̃ bands of Ar H²⁺: A joint theoretical/ experimental study. The Journal of Chemical Physics, 113, 2736–2740. Retrieved from http://scitation.aip.org/content/aip/journal/jcp/113/7/10.1063/1.1305263
http://dx.doi.org/10.1063/1.1305263
Brinkmann, N. R., Tschumper, G. S., & Schaefer, H. F. (1999). Electron affinities of the oxides of aluminum, silicon, phosphorus, sulfur, and chlorine. The Journal of Chemical Physics, 110, 6240–6245. Retrieved from http://www.researchgate.net/publication/6500864_Kinetics_of_sulfur_oxide_sulfur_fluoride_and_sulfur_oxyfluoride_anions_with_atomic_species_at_298_and_500_K http://dx.doi.org/10.1063/1.478528
Clark, T., Chandrasekhar, J., Spitznagel, G. W., & Schleyer, P. V. R. (1983). Efficient diffuse function-augmented basis sets for anion calculations. III. The 3-21G basis set for first-row elements, Li–F. Journal of Computational Chemistry, 4, 294–301. Retrieved from http://onlinelibrary.wiley.com/doi/10.1002/jcc.5400400303/abstract http://dx.doi.org/10.1002/jcc.5400400303
Curtiss, L. A., Raghavachari, K., Trucks, G. W., & Pople, J. A. (1991). Gaussian-2 theory for molecular energies of first- and second-row compounds. The Journal of Chemical Physics, 94, 7221–7230. Retrieved from http://www.researchgate.net/publication/234983938_Gaussian2_theory_using_reduced_MllerPlesset_orders http://dx.doi.org/10.1063/1.460205
Drowart, J., Myers, C. E., Szwarz, R., Vander Auwer-Mahieu, A., & Uy, O. M. (1973). The dissociation energies of the molecules PS, PSe, and PTe. High Temperature Science, 5, 482–488.
Dunning, T. H. (1989). Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen. The Journal of Chemical Physics, 90, 1007–1023. Retrieved from http://scitation.aip.org/content/aip/journal/jcp/90/2/10.1063/1.456153 http://dx.doi.org/10.1063/1.456153
Dyke, J. M., Morris, A., & Ridha, A. (1982). Study of the ground
state of PO+ using photoelectron spectroscopy. Journal of the Chemical Society, Faraday Transactions 2, 78, 2077–2082. Retrieved from http://pubs.rsc.org/en/content/articlelanding/1982/F2/1/29828702082#!divAbstract

Frisch, M. J., Pople, J. A., & Binkley, J. S. (1984). Self-consistent molecular orbital methods 25. Supplementary functions for Gaussian basis sets. The Journal of Chemical Physics, 80, 3265–3269. Retrieved from http://scitation.aip.org/content/aip/journal/jcp/80/7/10.1063/1.447079

Huber, K. P., & Herzberg, G. (1979). Molecular spectra and molecular structure. Van Nostrand Reinhold. Retrieved from http://link.springer.com/chapter/10.1007%2F978-1-4757-0961-2#page-2

Kroto, H. W., Nixon, J. F., & Ohno, K. (1981). The microwave spectrum of phosphabutadiyne, H–C–C–C–P. Journal of Molecular Spectroscopy, 90, 512–516. Retrieved from http://www.sciencedirect.com/science/article/pii/002228528190134X

Metropoulos, A., Papakondylis, A., & Movides, A. (2003). Ab initio investigation of the ground state properties of PO+, PO− and PO. The Journal of Chemical Physics, 119, 5981–5987. Retrieved from http://scitation.aip.org/content/aip/journal/jcp/119/12/10.1063/1.1599341

Müller, H. S. F., & Woon, D. E. (2013). Calculated dipole moments for silicon and phosphorus compounds of astrophysical interest. The Journal of Physical Chemistry A, 117, 13868–13877. Retrieved from http://pubs.acs.org/doi/abs/10.1021/jp4083807

Woon, D. E., & Dunning, T. H. (1993). Gaussian basis sets for use in correlated molecular calculations. III. The atoms aluminum through argon. The Journal of Chemical Physics, 98, 1358–1371. Retrieved from http://scitation.aip.org/content/aip/journal/jcp/98/2/10.1063/1.464303

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