

Triethylammonium salt of dimethyl diphenyldithiophosphates: Single crystal X-ray and DFT analysis

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MS received 3 December 2015; accepted 29 March 2016

Abstract. The present work demonstrates the single crystal X-ray and DFT analysis of $[(2,4\text{-CH}_3)_2\text{C}_6\text{H}_3\text{O}]_2\text{PS}_2\text{HNEt}_3$ (**1**) and $[(3,4\text{-CH}_3)_2\text{C}_6\text{H}_3\text{O}]_2\text{PS}_2\text{HNEt}_3$ (**2**) along with computational analysis of $[(3,5\text{-CH}_3)_2\text{C}_6\text{H}_3\text{O}]_2\text{PS}_2\text{HNEt}_3$ (**3**) by using density functional theory (DFT) in its hybrid form B3LYP method. Compounds **1** and **2** crystallize in the orthorhombic space group *Pbca* and triclinic space group *P1*, respectively and their X-ray analysis reveals that phosphorus atom is coordinated to the two S and two O atoms to form tetrahedral geometry. The structure is stabilized by cation–anion N–H...S hydrogen bonded interactions. The structural parameters, vibrational bands and energy gaps of frontier orbitals (HOMO–LUMO) have been calculated. The calculated geometric and spectral results matched the experimental data with good agreement. Theoretically calculated frontier molecular orbitals (HOMO–LUMO) and their energies suggest that charge transfer occurs within the compounds.

Keywords. Diphenyldithiophosphate; DFT; Single crystal X-ray; IR; HOMO-LUMO

1. Introduction

O, *O'*-Dialkyl- and alkylenedithiophosphates are extensively studied in which the ligands exhibited remarkable diversities in organic derivatives and their coordination pattern with the metals.^{1–6} These soft donor ligands are versatile ligands which show both chelating bidentate^{7,8} and less common monodentate linkage.^{9,10} The importance of metal dithiophosphates in petroleum industry as an oil additive^{11,12} and in agriculture¹³ as pesticides are well known. Recently, synthesis and characterization of ditolyldithiophosphates added a new extension in the area of dithiophosphate chemistry.^{14,15} These new ditolyldithiophosphate ligands appear to be potential chelating ligands to the metals, metalloids and non-metals akin to the dialkyl- and alkylenedithiophosphate ligands. Some metal complexes with the ditolyldibenzyl dithiophosphate ligands have also been reported.^{16–24} In our laboratory, we were successful in isolating a number of triethylammonium salt of disubstituted diphenyldithiophosphates²⁵ and their metal derivatives.²⁶ The

literature survey reveals only a few reports of theoretical calculations on the structural and vibrational properties of dithiophosphates.^{27,28} To the best of our knowledge, reports on theoretical calculations of ditolyldiphenyldithiophosphates have not been described so far. In order to comprehend and understand the experimental studies and to provide better insight into molecular parameters and vibrational spectra of the compounds, a comparison of computed structural and spectroscopic data with the previously reported experimental (crystallographic and spectroscopic) results has been investigated for the title compounds. The present work describes the crystal structures and DFT analyses of previously reported triethylammonium salt of disubstituted diphenyldithiophosphates.²⁵

2. Experimental

2.1 Crystallography data collection and refinement

Crystallization of compounds $[(2,4\text{-CH}_3)_2\text{C}_6\text{H}_3\text{O}]_2\text{PS}_2\text{HNEt}_3$ (**1**) and $[(3,4\text{-CH}_3)_2\text{C}_6\text{H}_3\text{O}]_2\text{PS}_2\text{HNEt}_3$ (**2**) was executed by very slow evaporation of their

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saturated solution in chloroform/n-hexane mixture (3:1) at room temperature which yielded suitable single crystals for X-ray analysis. X-ray data of compound **1** was collected on a Bruker Apex-II CCD diffractometer (Department of Chemistry, Guru Nanak Dev University, Amritsar) using Mo K α ($\lambda = 0.71069 \text{ \AA}$) at room temperature. The data were processed by SAINT correcting for Lorentz and polarization effects. An empirical absorption correction was applied using SADABS.²⁹ The solution was obtained by direct methods, using SIR-92³⁰ and refined by full-matrix least squares refinement methods³¹ based on F^2 , using SHELX-97. All non-hydrogen atoms were refined anisotropically. All calculations were performed using Wingx package.³² X-ray data of compound **2** was collected on an X'calibur-Oxford Diffraction single crystal diffractometer (Department of Physics and Electronics, University of Jammu, Jammu) with CCD area-detector (graphite-monochromator, Mo-K α radiations, $\lambda = 0.71073 \text{ \AA}$). Data were corrected for Lorentz, polarization and absorption factors. The structures were solved by direct methods using SHELXS97.³¹ All non-H atoms were located in the best E-map. Full-matrix least-squares refinement was carried out using SHELXL97.³¹ The geometry of the molecule was calculated using WinGX,³³ PARST³³ and PLATON.³⁴ Atomic scattering factors were taken from the International Tables for X-ray Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4). Molecular drawings were obtained using DIAMOND

version 2.1.³⁵ Crystallographic data, details of the data collection, structure solution and refinements are listed in table 1.

2.2 Computational details

The quantum chemical calculations (DFT calculations) giving molecular geometries of minimum energies, molecular orbitals (HOMO–LUMO) and vibrational spectra were performed using the Gaussian 03 package.³⁶ Molecular orbitals are visualized using “Gauss view”. The method used was Becke’s three-parameter hybrid-exchange functional, the nonlocal correlation provided by the Lee, Yang and Parr expression, and the Vosko, Wilk, and Nuair 1980 local correlation functional (III) (B3LYP).³⁷ The 6-31G*(d,p) basis set was used for C, N, O, P and S atoms. The input coordinates are obtained from the crystal structure data. The structural parameters were adjusted until an optimal agreement between calculated and experimental structure obtained throughout the entire range of available structures. Structural parameters obtained from the already reported crystal structures²⁵ were compared with those of optimized geometries. DFT study of number of metal complexes and compounds have been carried out with this DFT/B3LYP/6-31G*/LANL2DYZ method and found to be suitable for this study and to produce the experimental results.³⁸

Table 1. Summary of the crystal structure, data collection and structure refinement parameters for compounds **1** and **2**.

Compound	1	2
Chemical formula	C ₁₆ H ₁₈ O ₂ PS ₂ ·C ₆ H ₁₆ N	C ₁₆ H ₁₈ O ₂ PS ₂ ·C ₆ H ₁₆ N
M_r	439.61	439.61
Crystal system, space group	Orthorhombic, <i>Pbca</i>	Triclinic, <i>P1</i>
Temperature (K)	100	296
a, b, c (Å)	9.1400(4), 15.5853(8), 32.8880(15)	7.5104(8), 7.8179(8), 10.5067(11)
α, β, γ (°)	90.00, 90.00, 90.00	86.392(9), 85.285(9), 87.164(8)
V (Å ³)	4684.9(4)	612.99(11)
Z	8	1
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm ⁻¹)	0.31	0.30
Crystal size (mm)	0.11 × 0.08 × 0.06	0.30 × 0.20 × 0.20
Diffractometer	Bruker APEX-II CCD diffractometer	Xcalibur, Sapphire3 diffractometer
Absorption correction	Multi-scan	Multi-scan
T_{\min}, T_{\max}	0.678, 0.747	0.904, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	39777, 9788, 6551	4318, 2404, 2041
R_{int}	0.048	0.032
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.797	0.617
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.047, 0.126, 0.96	0.056, 0.154, 1.05
No. of reflections	9788	2404
No. of parameters	256	261
No. of restraints	1	4
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.49, -0.35	0.66 -0.28

3. Results and Discussion

3.1 Crystal and molecular structures of compounds **1** and **2**

The compounds **1** and **2** were crystallized in the orthorhombic space group *Pbca* and triclinic space group *P1*, respectively. Selected bond distances and bond angles for the compounds **1** and **2** are listed in tables **2** and **3**.

A distorted tetrahedral environment around phosphorus can be clearly seen with two sulfurs and two oxygens bonded to phosphorus (figure 1). The compounds **1** and **2** consist of triethylammonium and dithiophosphate moiety which are connected through N–H···S (table 4) intermolecular hydrogen bond. The N–S bond distances for compounds **1** and **2** are 3.185(1) and 3.337(5) Å which compare well with the value of (3.248(6) Å) reported³⁹ for [Et₃NH]⁺[(OCH₂CMe₂CH₂O)PS₂][−]. The values for the remaining hydrogen bonding parameters in compounds **1** and **2** of H···S are 2.33 and 2.57

Table 2. Selected experimental and calculated bond lengths (Å) and angles (°) for compound **1**.

Bond lengths/ Bond angles	Experimental	Calculated	Deviation
N1—H1	0.881(13)	0.950	−0.069
O1—P1	1.6279(10)	1.678	−0.050
O2—P1	1.6140(10)	1.661	−0.047
P1—S1	1.9413(5)	2.014	−0.073
P1—S2	1.9779(5)	1.989	−0.012
O2—P1—S2	110.17(4)	109.16	1.01
O1—P1—S2	108.91(4)	107.78	1.13
S1—P1—S2	118.46(2)	118.97	−0.51
O2—P1—O1	96.76(5)	96.05	0.71
O2—P1—S1	108.06(4)	107.78	0.28
O1—P1—S1	112.30(4)	111.63	0.67

Table 3. Selected experimental and calculated bond lengths (Å) and angles (°) for compound **2**.

Bond lengths/ Bond angles	Experimental	Calculated	Deviation
N1—H1A	0.87(5)	0.717	0.153
O1—P1	1.621(4)	1.607	0.014
O2—P1	1.606(4)	1.622	−0.016
P1—S2	1.9440(18)	1.961	−0.017
P1—S1	1.9626(18)	1.944	0.0186
O2—P1—S1	104.79(17)	111.82	−7.03
O1—P1—S1	110.37(16)	113.82	−3.45
S2—P1—S1	117.94(9)	117.94	0
O2—P1—O1	95.7(2)	95.67	0.03
O2—P1—S2	113.85(17)	110.38	3.47
O1—P1—S2	111.82(16)	104.78	7.04

Å and N–H···S are 162° and 149°, respectively, compared to (2.44 Å and 160°).³⁹ It is clear that the sulfur atoms, involved in hydrogen bonding, have the longer P–S bonds (1.9779(7) Å and 1.9626(18) Å) in compounds **1** and **2** whereas the sulfur atoms not involved in hydrogen bonding have shorter the S–P bonds lengths (1.9413(5) and 1.9440(18) Å). These bond lengths are longer than the terminal P=S bonds observed in HS₂POCMe₂CMe₂O and HS₂POCH₂CMe₂CH₂O (1.923(2) and 1.908(2) Å),⁴⁰ respectively, but shorter than those of K₂⁺[(MeO)OPS₂][−]·H₂O (2.007(6) and 2.011(5) Å),⁴¹ which is reflecting their partial double bond character. The average P–O bond lengths in

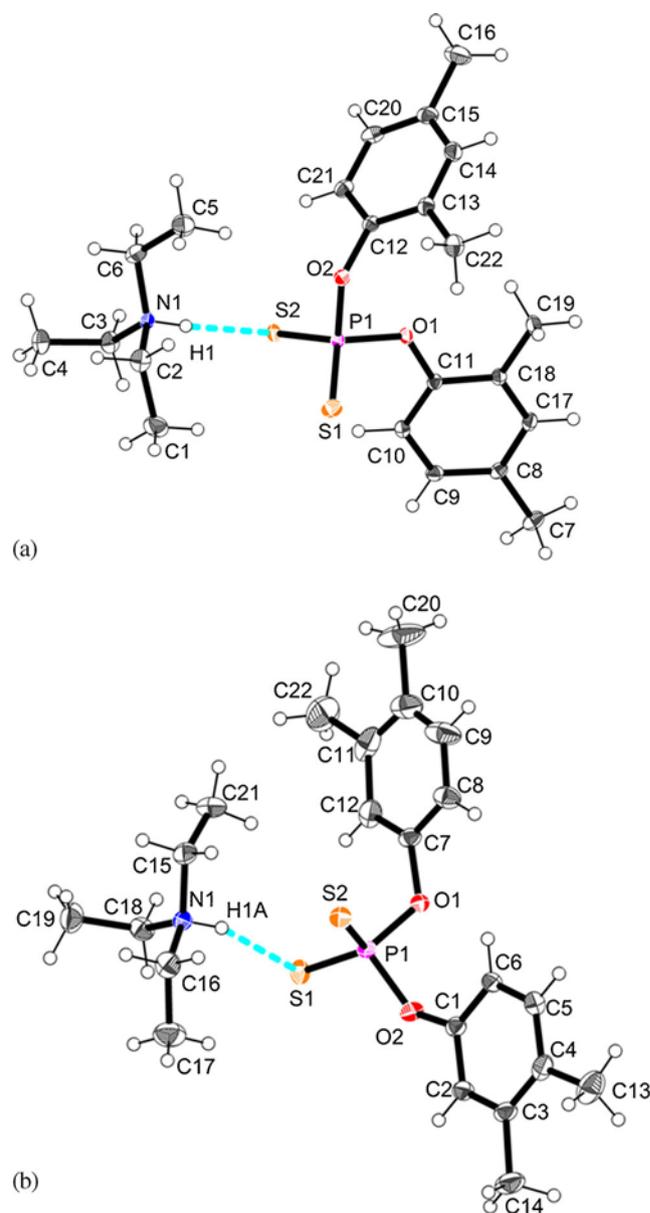


Figure 1. Molecular structure of (a) [(2,4-CH₃)₂C₆H₃O]₂PS₂HNEt₃ (**1**); (b) [(3,4-CH₃)₂C₆H₃O]₂PS₂HNEt₃ (**2**) with displacement ellipsoids drawn at 40% probability level.

Table 4. Selected hydrogen bonding interactions for compounds **1** and **2**.

Compound	D–H...A	H...A(Å)	D...A(Å)	D–H...A(°)
1	N1–H1...S2 ¹	2.334(16)	3.185(1)	162.54
2	N1–H1A...S1	2.57(4)	3.337(5)	149

Symmetry code: (i) x+1, +y, +z

compounds **1** and **2** are 1.620(10) and 1.613(4) Å which are similar to those of [Et₃NH]⁺[(2-MeC₆H₄O)₂PS₂][−] (1.622(2) Å).⁴² However, these bonds are slightly longer than that found in the free acids HS₂POCMe₂CMe₂O (1.5915(3) Å) and HS₂POCH₂CMe₂CH₂O (1.5825(3) Å).⁴⁰

The S–P–S bond angles for the compounds **1** and **2** are of 118.46(2)° and 117.94(9)° are akin to those in [Et₃NH]⁺[(2-MeC₆H₄O)₂PS₂][−] (118.62(4)°)⁴² but smaller than in [Et₃NH]⁺[CH₂{6-t-Bu-4-Me-C₆H₄O}₂P(S)(S)][−] (120.49(8)°)³⁹ while larger compared to the ligands HS₂POCMe₂CMe₂O (112.78(8)°), HS₂POCH₂CMe₂CH₂O (115.64(8)°)⁴⁰ and K₂⁺[(MeO)OPS₂][−].H₂O (113.67(3)°).⁴¹ The O–P–O bond angles of 96.76(5)° and 95.7(2)° in compounds **1** and **2** are similar to [Et₃NH]⁺[(2-MeC₆H₄O)₂PS₂][−] (97.07(8)°)⁴² but slightly larger in the compounds [Et₃NH]⁺[CH₂{6-t-Bu-4-Me-C₆H₄O}₂P(S)(S)][−] (103.5(4)°),³⁹ HS₂POCMe₂CMe₂O (105.1(1)°),⁴⁰ K₂⁺[(MeO)OPS₂][−].H₂O (100.93(7)°),⁴¹ and [Et₃NH]⁺[(OCH₂CMe₂CH₂O)₂PS₂][−] (101.4(2)°).³⁹

The N–H bond length in compounds **1** and **2** are 0.881(13) and 0.87(5) Å, which are in reasonable agreement with the values found in compound **3** (0.94(4) Å)²⁵ (table 3). P1–S1 and P1–S2 bond lengths for compound **1** are 1.9413(5) and 1.9779(5) Å while for compound **2**, bond lengths are 1.9440 (18) and 1.9626 (18) Å. These bond lengths are comparable with compound **3** (1.9389(12) and 1.9586(12) Å).²⁵ The S1–P1–S2 bond angle in compounds **1** and **2** is 118.46(2)° and 117.94(9)° which are akin to the value found in compound **3** (119.31(6)°).²⁵

3.2 Infrared spectra

Vibrational spectroscopy has been widely used for structural characterization of molecular systems by DFT calculations. It is found that the calculated frequencies by Gaussian 03 are closer to the experimental values. Experimental and calculated vibration frequencies along with corresponding vibrational assignments are given in table 5. IR spectra have shown a broad absorption for [νN–H] vibrations in the region 3431–3397 cm^{−1} in the compound **1-3** and the theoretical data for [νN–H] vibration is in the region 3651–3452 cm^{−1}. In the compounds **1-3** [ν(P)–O–C] and [νP–O–(C)] stretching vibrations were found in the region 1196–1141cm^{−1} and 870–843 cm^{−1}, respectively, which are in agreement with the results computed as 1196–1133 cm^{−1} and 895–845 cm^{−1} (for DFT). The observed bands in the region 688–672 cm^{−1} and 586–574 cm^{−1} for [νP=S] and [νP–S] match with the corresponding theoretical data and are found as 684–667 cm^{−1} and 575–542 cm^{−1}. In this study, only characteristic stretching vibration bands were identified which are in good agreement with the related experimental study previously reported.²⁵

3.3 Computational discussion

It would be appropriate here to correlate the structural parameters obtained from the crystal structure studies with computational data. Figure 2 shows the optimized molecular structures for compounds **1-3** for which comparison of the selected bond lengths and bond angles

Table 5. Selected experimental and calculated IR vibrational frequencies (cm^{−1}) for compounds **1-3**.

Assignment	Compound 1		Compound 2		Compound 3	
	Experimental	Theoretical	Experimental	Theoretical	Experimental	Theoretical
[νN–H]	3397 b	3651	3399 b	3452	3431 b	3488
[ν(P)–O–C]	1196 s	1196	1148 s	1154	1141 s	1133
[νP–O–(C)]	870 s	895	856 s	848	843 s	851
[νP=S]	673 s	684	672 s	686	688 s	667
[νP–S]	586 m	575	574 m	542	578 m	570

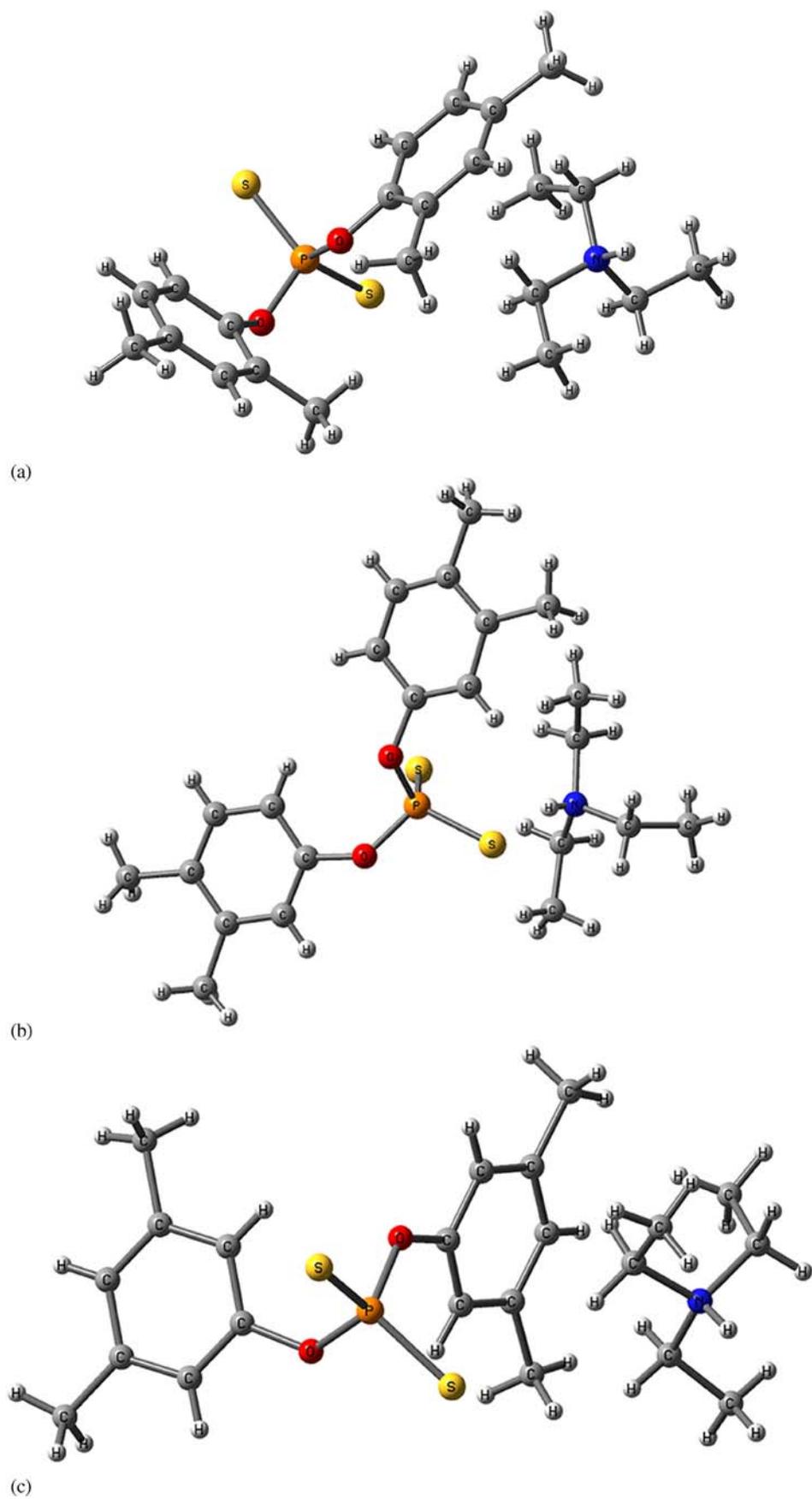


Figure 2. Optimized structure of, (a) $[(2,4\text{-CH}_3)_2\text{C}_6\text{H}_3\text{O}]_2\text{PS}_2\text{HNEt}_3$ (**1**); (b) $[(3,4\text{-CH}_3)_2\text{C}_6\text{H}_3\text{O}]_2\text{PS}_2\text{HNEt}_3$ (**2**); (c) $[(3,5\text{-CH}_3)_2\text{C}_6\text{H}_3\text{O}]_2\text{PS}_2\text{HNEt}_3$ (**3**).

Table 6. Selected experimental and calculated bond lengths (Å) and angles (°) for compound **3**.

Bond lengths/ Bond angles	Experimental	Calculated	Deviation
N1—H1	0.94(4)	0.94	0
P1—O1	1.610(2)	1.622	-0.012
P1—O2	1.622(2)	1.610	0.012
P1—S1	1.9389(12)	1.939	0.001
P1—S2	1.9586(12)	1.958	0
O1—P1—O2	102.33(12)	102.33	0
O1—P1—S1	112.57(10)	111.07	1.5
O2—P1—S1	105.96(9)	104.39	1.57
O1—P1—S2	104.41(9)	105.96	-1.55
O2—P1—S2	111.06(9)	112.57	1.51
S1—P1—S2	119.31(6)	119.31	0

are given in the tables 2, 3 and 6. Interestingly, all of the geometric structures were identified and after optimization they tend to reorganise close to the experimental structures. The optimized geometry analysis reveals that the observed and calculated coordination number and the molecular geometry are also in agreement. The computed bond lengths and bond angles help us to understand the molecular structure of the compounds. The experimental values for N-H bond lengths for compounds **1-3** (0.87(5)-0.94(4) Å) are comparable with computed bond lengths (0.717-0.950 Å). The experimental P1-S1 and P1-S2 bond lengths (1.9389(12)-1.9440(18) Å) and (1.9586(12)-1.9779(15) Å) are as good as the theoretical values (1.939-2.014 and 1.944-1.989 Å). The bond angle S1-P-S2 is measured as 117.94(9)-119.31(6)° and it is calculated as 117.95°-119.31° by using DFT.

3.4 HOMO-LUMO analyses

The frontier molecular orbital energies have been calculated with B3LYP/6-31G*/LANL2DZ level of theory in the gaseous phase. The HOMO and LUMO are main orbitals that take part in chemical reactions. It has been found that the HOMO is largely distributed over the oxygen and sulfur atoms of anionic dithiophosphates moiety in compounds **1-3**. LUMO, the lowest unoccupied molecular orbital, is distributed over the triethylammonium moiety in compounds **1** and **3** while it is distributed over the phenyl ring of dithiophosphate in compound **2** (figure 3). The energy gap between the HOMO and the LUMO is a critical parameter in determining molecular electrical transport properties and electron conductivity. The energy gap values in the compounds **1-3** are 3.952 eV, 4.575 eV and 4.0197 eV, respectively. Further, HOMO and LUMO

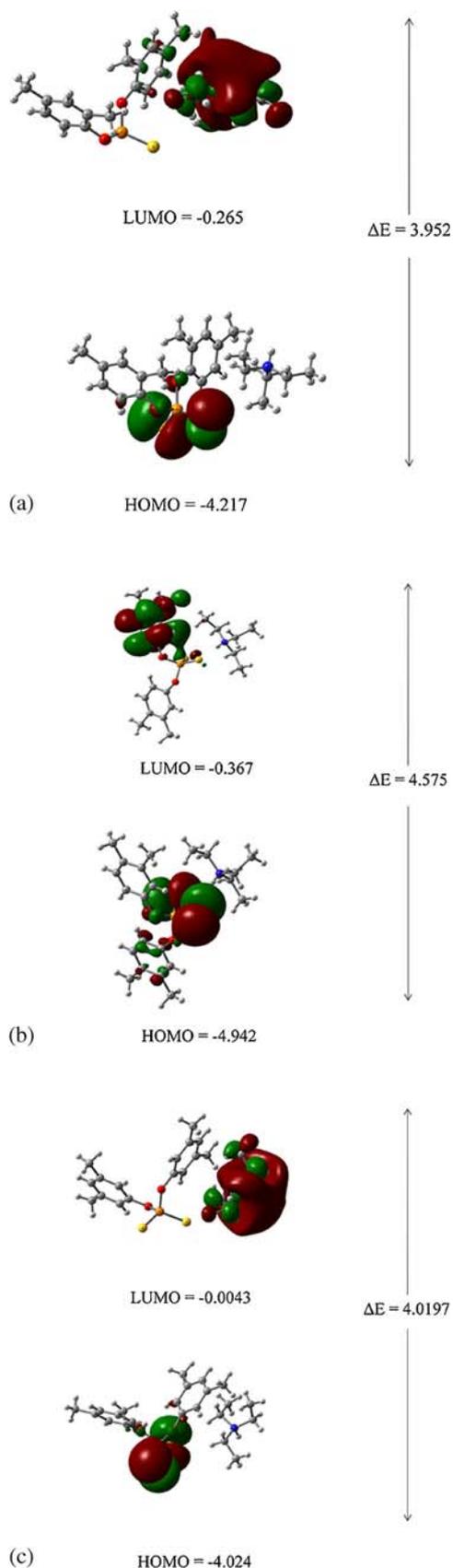


Figure 3. Frontier molecular orbital surfaces and energy gap for, (a) $[(2,4\text{-CH}_3)_2\text{C}_6\text{H}_3\text{O}]_2\text{PS}_2\text{HNEt}_3$ (**1**); (b) $[(3,4\text{-CH}_3)_2\text{C}_6\text{H}_3\text{O}]_2\text{PS}_2\text{HNEt}_3$ (**2**); (c) $[(3,5\text{-CH}_3)_2\text{C}_6\text{H}_3\text{O}]_2\text{PS}_2\text{HNEt}_3$.

energy gap also explains the eventual charge transfer interactions taking place within the molecule.⁴³

4. Conclusions

In the present work, DFT studies of the structure in terms of geometries, bond lengths and bond angles as well as spectroscopic properties (vibrational and HOMO–LUMO) of aromatic dithiophosphates are reported and compared with experimental results for the first time. X-ray analysis reveals that tetrahedral coordination around the phosphorus atom is formed by two S and two O atoms. The structure is stabilized by cation–anion N–H···S hydrogen bond interactions. The theoretical, experimental and vibrational structural parameters are in qualitative agreement with crystal and spectroscopic data. The experimental and theoretical bond lengths and angles are in good agreement with each other with small deviations. The accuracy of results also predicts that the DFT studies performed at B3LYP/LANL2DZ level is the appropriate quantum chemical method for reproducing the experimental results for these compounds. The small discrepancies in geometric and vibrational parameters are attributable to the packing interactions within the lattice which are not modelled in computational study. HOMO–LUMO gaps suggest that the charge transfer interactions occur within these complexes.

Supplementary Information (SI)

CCDC 1414793-1414794 contain the supplementary crystallographic data for compounds **1** and **2**. These data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/conts/retrieving.html>, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk.

Acknowledgements

RK acknowledges the DST for the single crystal X-ray diffractometer as a National Facility under Project No. SR/S2/CMP-47/2003.

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