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O-2-Naphthyl diphenylthiophosphinate

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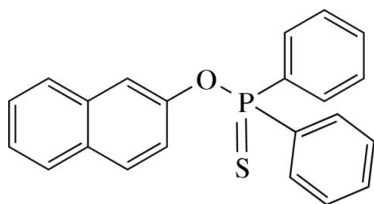
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.032; wR factor = 0.084; data-to-parameter ratio = 20.2.

The molecule of the title compound, $\text{C}_{10}\text{H}_7\text{OP}(\text{S})(\text{C}_6\text{H}_5)_2$ or $\text{C}_{22}\text{H}_{17}\text{OPS}$, exhibits distorted tetrahedral geometry about the P atom. The $\text{P}=\text{S}$ bond of 1.9355 (4) Å is shorter than that found in $\text{Ph}_3\text{P}=\text{S}$ [1.950 (3) Å] because the replacement of one carbon on phosphorus by oxygen increases the effective electronegativity of the P atom, thereby enhancing $p\pi-d\pi$ back-donation from a lone-pair orbital of the S atom.

Related literature

For general background, see: Aragoni *et al.* (1999); Boyle & Godfrey (2001); Ferraro & Williams (1987); Zingaro (1963); Cross *et al.* (1999); Schweikert & Meyers (1968); Laurence *et al.* (1998); Zingaro & Hedges (1961); Arca *et al.* (1999). For a related structure, see: Coddling & Kerr (1978); Mague *et al.* (2007).



Experimental

Crystal data

$\text{C}_{22}\text{H}_{17}\text{OPS}$
 $M_r = 360.39$
 Monoclinic, $P2_1/n$
 $a = 9.7701$ (3) Å
 $b = 19.1380$ (6) Å
 $c = 9.8933$ (3) Å
 $\beta = 105.834$ (1)°

$V = 1779.7$ (1) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.28$ mm⁻¹
 $T = 100$ (2) K
 $0.24 \times 0.16 \times 0.13$ mm

Data collection

Bruker SMART APEX II CCD
 area-detector diffractometer

Absorption correction: multi-scan
 (SADABS; Sheldrick, 2007)
 $T_{\min} = 0.908$, $T_{\max} = 0.966$

31295 measured reflections
 4573 independent reflections

4083 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.084$
 $S = 1.05$
 4573 reflections

226 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.36$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.35$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

S1—P1	1.9355 (4)		
O1—P1—C17	97.71 (5)	C17—P1—S1	114.00 (4)
O1—P1—C11	103.32 (5)	C11—P1—S1	115.15 (4)
C17—P1—C11	108.43 (5)	C1—O1—P1	126.61 (8)
O1—P1—S1	116.37 (4)		

Data collection: APEX2 (Bruker, 2007); cell refinement: APEX2; data reduction: SAINT-Plus (Bruker, 2006); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: APEX2 (Bruker, 2007); software used to prepare material for publication: APEX2.

We thank the Chemistry Department of Tulane University for support of the X-ray laboratory and the Louisiana Educational Quality Support Fund, administered by the Louisiana Board of Regents, for purchase of the CCD diffractometer under Grant LEQSF (2002–03)-ENH-TR-67. Financial support by the Department of Science and Technology (DST) and the Council of Scientific and Industrial Research (CSIR), New Delhi, India, is also gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2358).

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supplementary materials

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O-2-Naphthyl diphenylthiophosphinate

J. T. Mague, B. Punji, C. Ganesamoorthy and M. S. Balakrishna

Comment

During the past few decades, charge transfer (CT) compounds have been the subject of extensive structural and theoretical investigations because they can be used in fields as diverse as medicine, electronics and synthetic organic and inorganic chemistry (see, *e.g.* Ferraro & Williams (1987), Laurence *et al.* (1998), Aragoni *et al.* (1999) and Boyle & Godfrey (2001)). The ability of tertiary phosphine chalcogenides to form CT compounds with dihalogens and interhalogens was first reported by Zingaro (Zingaro & Hedges (1961), Zingaro (1963)). Recently, several groups have begun to investigate the role of phosphine chalcogenide CT compounds in the above areas (see, *e.g.* Cross *et al.* (1999) and Arca *et al.* (1999)). In the case of tertiary phosphine selenides, reaction with IX ($X = \text{Cl, Br or I}$) appeared to produce the CT compounds $R_3\text{PSe-I-X}$. In the case of the interhalogen complexes it is the heavier halogen which binds to the selenium atom. For trialkylphosphine sulfides, a similar result is observed *i.e.* 1:1 C T complex formation upon reaction with IX ($X = \text{Cl, Br or I}$). However in the reaction of triphenylphosphine sulfide with excess diiodine, an unusual 2:3 ($2\text{Ph}_3\text{PS}\cdot 3\text{I}_2$) adduct was isolated (Schweikert & Meyers, 1968). In these CT complexes, electron density on the $R_3\text{PE}$ ($E = \text{S or Se}$) moiety is donated to the σ^* antibonding orbitals of the X_2 molecule thus causing a lengthening of the $X-X$ bond compared to that of the free halogen. This is greater in the selenide CT complex than in the sulfide analog because of the greater donor power of selenium compared to sulfur. The $X-X$ bond length in the CT complexes is also sensitive to the nature of substituents on the phosphorus atom. The present study is part of a structural investigation of phosphine chalcogenide ligands directed at obtaining a better understanding of the factors that influence bonding in these molecules which in turn may help predict the type of CT compounds they may form.

A perspective view of the title compound is shown in Fig. 1. The distorted tetrahedral geometry about phosphorus is evidenced by the angles at phosphorus which range from $97.71(5)^\circ$ (O1-P1-C17) to $116.4(5)^\circ$ (O1-P1-S1). The $\text{P}=\text{S}$ bond of $1.9355(4) \text{ \AA}$ (Table 1) is shorter than that in $\text{Ph}_3\text{P}=\text{S}$ ($1.950(3) \text{ \AA}$ (Coddling & Kerr, 1978)) because the replacement of one carbon on phosphorus by oxygen increases the effective electronegativity of the phosphorus atom thereby enhancing $p\pi-d\pi$ back donation from a lone pair orbital of the sulfur atom and shortens the $\text{P}=\text{S}$ bond. In the title compound the dihedral angles between the mean plane of the naphthyl group and the mean planes of the phenyl rings built on C11 and C17 are, respectively, $79.94(5)$ and $56.21(5)^\circ$ while that between the mean planes of the phenyl rings is $68.97(6)^\circ$. The P1-O1-C1-C2 torsion angle is $171.64(9)^\circ$.

Experimental

A mixture of $\text{C}_{10}\text{H}_7\text{OPPh}_2$ (1 g, 3.04 mmol) and elemental sulfur (0.097 g, 3.04 mmol) in toluene (20 ml) was heated at 90°C for about 10 minutes. The mixture was cooled to room temperature and the solvent removed *in vacuo* to yield a pasty liquid which was dissolved in CH_2Cl_2 and layered with petroleum ether. Colorless crystals of the title compound formed on standing overnight at 0°C . Yield: 76% (0.83 g). Anal. Calcd. for $\text{C}_{22}\text{H}_{17}\text{OPS}$: C, 73.32; H, 4.75; S, 8.89%. Found: C, 73.19; H, 4.61; S, 8.76%.

Refinement

H atoms were placed in calculated positions with C—H = 0.95 Å and refined as riding contributions with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

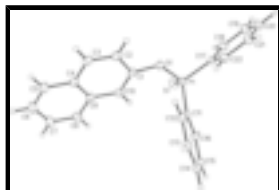


Fig. 1. Perspective view of I. Displacement ellipsoids are drawn at the 50% probability level and H-atoms are represented by spheres of arbitrary radius.

O-2-Naphthyl diphenylthiophosphate

Crystal data

$\text{C}_{22}\text{H}_{17}\text{OPS}$

$M_r = 360.39$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 9.7701(3) \text{ \AA}$

$b = 19.1380(6) \text{ \AA}$

$c = 9.8933(3) \text{ \AA}$

$\beta = 105.834(1)^\circ$

$V = 1779.7(1) \text{ \AA}^3$

$Z = 4$

$F_{000} = 752$

$D_x = 1.345 \text{ Mg m}^{-3}$

Melting point: 373-375 K

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 9913 reflections

$\theta = 2.4\text{--}29.4^\circ$

$\mu = 0.28 \text{ mm}^{-1}$

$T = 100(2) \text{ K}$

Block, colourless

$0.24 \times 0.16 \times 0.13 \text{ mm}$

Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 100(2) \text{ K}$

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2007)

$T_{\text{min}} = 0.908$, $T_{\text{max}} = 0.966$

31295 measured reflections

4573 independent reflections

4083 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\text{max}} = 28.7^\circ$

$\theta_{\text{min}} = 2.4^\circ$

$h = -13 \rightarrow 13$

$k = -25 \rightarrow 25$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.032$$

$$wR(F^2) = 0.084$$

$$S = 1.05$$

4573 reflections

226 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 0.8993P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.36 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.35 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5 °. in omega, collected at phi = 0.00, 90.00 and 180.00 °. and 2 sets of 800 frames, each of width 0.45 ° in phi, collected at omega = -30.00 and 210.00 °. The scan time was 15 sec/frame.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	-0.08033 (3)	0.849586 (17)	0.01116 (3)	0.02282 (9)
P1	0.10022 (3)	0.816997 (15)	0.12964 (3)	0.01521 (8)
O1	0.09681 (9)	0.78019 (5)	0.27593 (9)	0.01828 (17)
C1	0.02383 (12)	0.71931 (6)	0.29126 (12)	0.0169 (2)
C2	0.05707 (13)	0.69478 (7)	0.43088 (13)	0.0201 (2)
H2	0.1247	0.7189	0.5031	0.024*
C3	-0.00811 (14)	0.63626 (7)	0.46202 (13)	0.0220 (2)
H3	0.0156	0.6194	0.5559	0.026*
C4	-0.11095 (13)	0.60028 (6)	0.35561 (13)	0.0202 (2)
C5	-0.17985 (15)	0.53896 (7)	0.38492 (15)	0.0258 (3)
H5	-0.1578	0.5214	0.4782	0.031*
C6	-0.27766 (15)	0.50503 (7)	0.28000 (16)	0.0293 (3)
H6	-0.3230	0.4641	0.3008	0.035*
C7	-0.31155 (14)	0.53064 (7)	0.14100 (16)	0.0276 (3)
H7	-0.3793	0.5066	0.0688	0.033*
C8	-0.24774 (13)	0.58994 (7)	0.10886 (14)	0.0221 (2)
H8	-0.2724	0.6069	0.0150	0.026*
C9	-0.14487 (12)	0.62608 (6)	0.21541 (13)	0.0178 (2)
C10	-0.07381 (12)	0.68640 (6)	0.18446 (12)	0.0175 (2)

supplementary materials

H10	-0.0938	0.7036	0.0910	0.021*
C11	0.19044 (12)	0.75353 (6)	0.04975 (12)	0.0161 (2)
C12	0.28582 (13)	0.70621 (6)	0.13399 (13)	0.0194 (2)
H12	0.2988	0.7058	0.2327	0.023*
C13	0.36164 (14)	0.65980 (7)	0.07347 (15)	0.0240 (3)
H13	0.4275	0.6282	0.1309	0.029*
C14	0.34077 (15)	0.65982 (7)	-0.07084 (15)	0.0257 (3)
H14	0.3932	0.6285	-0.1120	0.031*
C15	0.24383 (14)	0.70530 (7)	-0.15556 (13)	0.0242 (3)
H15	0.2283	0.7041	-0.2546	0.029*
C16	0.16905 (13)	0.75275 (7)	-0.09583 (12)	0.0197 (2)
H16	0.1039	0.7844	-0.1538	0.024*
C17	0.22356 (12)	0.88595 (6)	0.20284 (12)	0.0171 (2)
C18	0.17919 (14)	0.95549 (7)	0.18510 (13)	0.0217 (2)
H18	0.0849	0.9665	0.1323	0.026*
C19	0.27334 (16)	1.00869 (7)	0.24487 (14)	0.0261 (3)
H19	0.2431	1.0560	0.2336	0.031*
C20	0.41147 (15)	0.99270 (7)	0.32104 (14)	0.0260 (3)
H20	0.4755	1.0292	0.3615	0.031*
C21	0.45647 (14)	0.92363 (7)	0.33830 (14)	0.0251 (3)
H21	0.5512	0.9130	0.3903	0.030*
C22	0.36292 (13)	0.87011 (7)	0.27945 (13)	0.0211 (2)
H22	0.3936	0.8228	0.2913	0.025*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01632 (14)	0.02408 (16)	0.02361 (16)	0.00217 (11)	-0.00211 (11)	0.00061 (12)
P1	0.01376 (14)	0.01647 (15)	0.01412 (14)	-0.00038 (10)	0.00165 (10)	-0.00012 (10)
O1	0.0185 (4)	0.0213 (4)	0.0147 (4)	-0.0040 (3)	0.0042 (3)	-0.0005 (3)
C1	0.0157 (5)	0.0186 (5)	0.0175 (5)	0.0007 (4)	0.0067 (4)	0.0004 (4)
C2	0.0191 (5)	0.0243 (6)	0.0163 (5)	0.0017 (4)	0.0038 (4)	-0.0009 (4)
C3	0.0256 (6)	0.0251 (6)	0.0166 (6)	0.0037 (5)	0.0077 (5)	0.0036 (5)
C4	0.0215 (6)	0.0195 (6)	0.0223 (6)	0.0036 (4)	0.0106 (5)	0.0023 (4)
C5	0.0309 (7)	0.0220 (6)	0.0294 (7)	0.0017 (5)	0.0164 (5)	0.0048 (5)
C6	0.0292 (7)	0.0214 (6)	0.0414 (8)	-0.0037 (5)	0.0163 (6)	0.0025 (6)
C7	0.0218 (6)	0.0242 (6)	0.0362 (8)	-0.0037 (5)	0.0069 (5)	-0.0022 (5)
C8	0.0193 (6)	0.0220 (6)	0.0242 (6)	-0.0003 (5)	0.0047 (5)	-0.0004 (5)
C9	0.0158 (5)	0.0179 (5)	0.0210 (6)	0.0022 (4)	0.0071 (4)	-0.0006 (4)
C10	0.0173 (5)	0.0197 (6)	0.0159 (5)	0.0008 (4)	0.0052 (4)	0.0010 (4)
C11	0.0159 (5)	0.0159 (5)	0.0164 (5)	-0.0027 (4)	0.0040 (4)	-0.0011 (4)
C12	0.0217 (6)	0.0184 (6)	0.0183 (6)	-0.0001 (4)	0.0056 (4)	0.0012 (4)
C13	0.0246 (6)	0.0171 (6)	0.0324 (7)	0.0014 (5)	0.0110 (5)	0.0003 (5)
C14	0.0284 (7)	0.0201 (6)	0.0337 (7)	-0.0065 (5)	0.0171 (6)	-0.0084 (5)
C15	0.0283 (6)	0.0284 (6)	0.0183 (6)	-0.0112 (5)	0.0105 (5)	-0.0073 (5)
C16	0.0200 (5)	0.0225 (6)	0.0157 (6)	-0.0060 (4)	0.0032 (4)	0.0000 (4)
C17	0.0171 (5)	0.0190 (6)	0.0152 (5)	-0.0022 (4)	0.0044 (4)	-0.0021 (4)
C18	0.0245 (6)	0.0199 (6)	0.0195 (6)	0.0005 (5)	0.0042 (5)	0.0000 (5)

C19	0.0376 (7)	0.0177 (6)	0.0230 (6)	-0.0034 (5)	0.0082 (5)	-0.0013 (5)
C20	0.0309 (7)	0.0269 (7)	0.0216 (6)	-0.0129 (5)	0.0099 (5)	-0.0061 (5)
C21	0.0177 (6)	0.0330 (7)	0.0241 (6)	-0.0052 (5)	0.0047 (5)	-0.0079 (5)
C22	0.0177 (5)	0.0221 (6)	0.0224 (6)	-0.0001 (4)	0.0039 (4)	-0.0047 (5)

Geometric parameters (Å, °)

S1—P1	1.9355 (4)	C11—C16	1.3979 (16)
P1—O1	1.6182 (9)	C11—C12	1.3996 (16)
P1—C17	1.8004 (12)	C12—C13	1.3923 (17)
P1—C11	1.8048 (12)	C12—H12	0.9500
O1—C1	1.3957 (14)	C13—C14	1.386 (2)
C1—C10	1.3685 (16)	C13—H13	0.9500
C1—C2	1.4103 (16)	C14—C15	1.387 (2)
C2—C3	1.3645 (18)	C14—H14	0.9500
C2—H2	0.9500	C15—C16	1.3941 (18)
C3—C4	1.4194 (18)	C15—H15	0.9500
C3—H3	0.9500	C16—H16	0.9500
C4—C5	1.4217 (18)	C17—C18	1.3959 (17)
C4—C9	1.4236 (17)	C17—C22	1.3990 (16)
C5—C6	1.368 (2)	C18—C19	1.3912 (18)
C5—H5	0.9500	C18—H18	0.9500
C6—C7	1.412 (2)	C19—C20	1.388 (2)
C6—H6	0.9500	C19—H19	0.9500
C7—C8	1.3732 (18)	C20—C21	1.389 (2)
C7—H7	0.9500	C20—H20	0.9500
C8—C9	1.4218 (17)	C21—C22	1.3904 (17)
C8—H8	0.9500	C21—H21	0.9500
C9—C10	1.4229 (16)	C22—H22	0.9500
C10—H10	0.9500		
O1—P1—C17	97.71 (5)	C16—C11—C12	119.65 (11)
O1—P1—C11	103.32 (5)	C16—C11—P1	120.32 (9)
C17—P1—C11	108.43 (5)	C12—C11—P1	120.00 (9)
O1—P1—S1	116.37 (4)	C13—C12—C11	120.17 (11)
C17—P1—S1	114.00 (4)	C13—C12—H12	119.9
C11—P1—S1	115.15 (4)	C11—C12—H12	119.9
C1—O1—P1	126.61 (8)	C14—C13—C12	119.79 (12)
C10—C1—O1	124.71 (10)	C14—C13—H13	120.1
C10—C1—C2	121.92 (11)	C12—C13—H13	120.1
O1—C1—C2	113.35 (10)	C13—C14—C15	120.46 (12)
C3—C2—C1	119.83 (11)	C13—C14—H14	119.8
C3—C2—H2	120.1	C15—C14—H14	119.8
C1—C2—H2	120.1	C14—C15—C16	120.20 (12)
C2—C3—C4	120.68 (11)	C14—C15—H15	119.9
C2—C3—H3	119.7	C16—C15—H15	119.9
C4—C3—H3	119.7	C15—C16—C11	119.69 (12)
C3—C4—C5	121.87 (12)	C15—C16—H16	120.2
C3—C4—C9	118.94 (11)	C11—C16—H16	120.2
C5—C4—C9	119.19 (12)	C18—C17—C22	119.85 (11)

supplementary materials

C6—C5—C4	120.58 (13)	C18—C17—P1	119.83 (9)
C6—C5—H5	119.7	C22—C17—P1	120.32 (9)
C4—C5—H5	119.7	C19—C18—C17	119.84 (12)
C5—C6—C7	120.27 (12)	C19—C18—H18	120.1
C5—C6—H6	119.9	C17—C18—H18	120.1
C7—C6—H6	119.9	C20—C19—C18	120.10 (12)
C8—C7—C6	120.79 (13)	C20—C19—H19	119.9
C8—C7—H7	119.6	C18—C19—H19	119.9
C6—C7—H7	119.6	C19—C20—C21	120.31 (12)
C7—C8—C9	120.27 (12)	C19—C20—H20	119.8
C7—C8—H8	119.9	C21—C20—H20	119.8
C9—C8—H8	119.9	C20—C21—C22	119.99 (12)
C8—C9—C10	121.52 (11)	C20—C21—H21	120.0
C8—C9—C4	118.90 (11)	C22—C21—H21	120.0
C10—C9—C4	119.57 (11)	C21—C22—C17	119.91 (12)
C1—C10—C9	119.04 (11)	C21—C22—H22	120.0
C1—C10—H10	120.5	C17—C22—H22	120.0
C9—C10—H10	120.5		

Fig. 1

