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O-2-Naphthyl diphenylselenophosphinate

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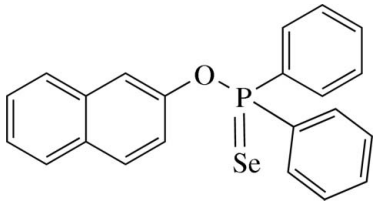
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.091; data-to-parameter ratio = 20.7.

The title compound, $C_{10}H_7OP(Se)(C_6H_5)_2$ or $C_{22}H_{17}OPSe$, is isomorphous and isostructural with its sulfur analog and shows a distorted tetrahedral geometry about the P atom. The P=Se bond of 2.0890 (5) Å is shorter than that of 2.106 (1) Å found in Ph_3P=Se 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 chalcogen atom and shortens the P=Se bond.

Related literature

For general background, see: Mague *et al.* (2007); Cross *et al.* (1999); Arca *et al.* (1999). For related structures, see: Mague *et al.* (2007); Codding & Kerr (1979).



Experimental

Crystal data

$C_{22}H_{17}OPSe$
M_r = 407.29
Monoclinic, $P2_1/n$
a = 9.9490 (8) Å
b = 19.044 (2) Å
c = 9.9552 (8) Å
β = 105.672 (1)°
V = 1816.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.16 mm^{-1}
T = 100 (2) K
0.26 × 0.24 × 0.15 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.545, T_{max} = 0.727
30965 measured reflections
4675 independent reflections
3896 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.091
S = 1.04
4675 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.95 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Se1—P1	2.0890 (5)		
O1—P1—C17	97.68 (8)	C17—P1—Se1	114.05 (7)
O1—P1—C11	103.29 (8)	C11—P1—Se1	115.41 (6)
C17—P1—C11	108.10 (9)	C1—O1—P1	126.43 (12)
O1—P1—Se1	116.37 (5)		

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*; software used to prepare material for publication: *APEX2*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2359).

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supplementary materials

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O-2-Naphthyl diphenylselenophosphinate

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Comment

During the past few decades, charge transfer (CT) compounds have been the subject of extensive structural and theoretical investigations (Mague *et al.*, 2007), and more 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)). 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 I is shown in Fig. 1. The distorted tetrahedral geometry about phosphorus is evidenced by the angles at phosphorus which range from 97.68 (8)° (O1—P1—C17) to 116.37 (5)° (O1—P1—Se1). The P═Se bond of 2.0890 (5) Å (Table 1) is shorter than 2.106 (1) Å found in Ph_3P=Se (Codding & Kerr, 1979) because the replacement of one carbon on phosphorus by oxygen increases the effective electronegativity of the phosphorus atom thereby enhancing pπ-dπ back donation from a lone pair orbital of the chalcogen atom and shortens the P═Se bond. In the title compound the dihedral angles between the mean plane of the naphthyl group and mean planes of the phenyl rings built on C11 and C17 are, respectively, 80.97 (7) and 56.88 (7)° while that between the mean planes of the phenyl rings is 70.15 (8)°. The P1—O1—C1—C2 torsion angle is 173.8 (1)°.

Experimental

A mixture of $C_{10}H_7OPPh_2$ (1 g, 3.04 mmol) and elemental selenium (0.24 g, 3.04 mmol) in toluene (20 ml) was heated to reflux for 10 h and was then cooled to room temperature. It was then filtered 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 were formed on standing overnight at 0 °C. Yield: 91% (1.12 g). Anal. Calcd. for $C_{22}H_{17}OPSe$: C, 64.87; H, 4.21%. Found: C, 64.63; H, 4.13%.

Refinement

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

Figures

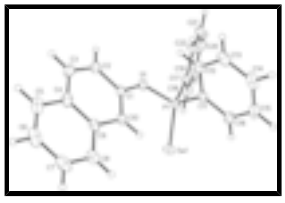


Fig. 1. Perspective view of I. Displacement ellipsoids are drawn at the 50% probability level and H-atoms are represented by spheres of arbitrary radius.

O-2-Naphthyl diphenylselenophosphinate

Crystal data

$C_{22}H_{17}OPSe$	F_{000} = 824
M_r = 407.29	D_x = 1.490 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 391-393 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 9.9490 (8) Å	Cell parameters from 9901 reflections
b = 19.044 (2) Å	θ = 2.4–29.2º
c = 9.9552 (8) Å	μ = 2.16 mm^{-1}
β = 105.672 (1)º	T = 100 (2) K
V = 1816.1 (3) Å^3	Block, colourless
Z = 4	0.26 × 0.24 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	4675 independent reflections
Radiation source: fine-focus sealed tube	3896 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.036
T = 100(2) K	θ_{max} = 28.8º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 2007)	h = −13→13
T_{min} = 0.545, T_{max} = 0.727	k = −25→25
30965 measured reflections	l = −13→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.033	H-atom parameters constrained
$wR(F^2)$ = 0.091	$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.981P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
4675 reflections	$\Delta\rho_{max}$ = 0.95 e Å^{-3}
226 parameters	$\Delta\rho_{min}$ = −0.61 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5 °. in omega, colllected 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 10 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 $F^2 > 2\text{sigma}(F^2)$ 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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Se1	0.49213 (2)	0.142334 (11)	0.58260 (2)	0.02478 (8)
P1	0.36997 (5)	0.18120 (3)	0.39250 (5)	0.01726 (11)
O1	0.22562 (14)	0.21964 (7)	0.39571 (14)	0.0206 (3)
C1	0.21246 (19)	0.27988 (10)	0.4718 (2)	0.0192 (4)
C2	0.0736 (2)	0.30497 (12)	0.4418 (2)	0.0229 (4)
H2	0.0012	0.2816	0.3746	0.027*
C3	0.0441 (2)	0.36264 (11)	0.5095 (2)	0.0258 (4)
H3	−0.0489	0.3799	0.4879	0.031*
C4	0.1507 (2)	0.39731 (11)	0.6119 (2)	0.0231 (4)
C5	0.1234 (2)	0.45743 (12)	0.6846 (3)	0.0309 (5)
H5	0.0312	0.4756	0.6646	0.037*
C6	0.2283 (3)	0.48944 (13)	0.7830 (3)	0.0352 (5)
H6	0.2085	0.5295	0.8313	0.042*
C7	0.3657 (3)	0.46325 (12)	0.8133 (2)	0.0321 (5)
H7	0.4380	0.4859	0.8816	0.038*
C8	0.3961 (2)	0.40536 (11)	0.7450 (2)	0.0252 (4)
H8	0.4891	0.3882	0.7667	0.030*
C9	0.2897 (2)	0.37103 (11)	0.6423 (2)	0.0208 (4)
C10	0.3189 (2)	0.31175 (10)	0.5677 (2)	0.0197 (4)
H10	0.4117	0.2946	0.5846	0.024*
C11	0.45437 (19)	0.24513 (10)	0.30831 (19)	0.0185 (4)
C12	0.3740 (2)	0.29457 (11)	0.2174 (2)	0.0219 (4)
H12	0.2760	0.2965	0.2051	0.026*
C13	0.4370 (2)	0.34104 (12)	0.1447 (2)	0.0276 (4)
H13	0.3820	0.3740	0.0817	0.033*
C14	0.5804 (2)	0.33876 (12)	0.1649 (2)	0.0293 (5)
H14	0.6236	0.3701	0.1151	0.035*
C15	0.6610 (2)	0.29102 (12)	0.2574 (2)	0.0279 (5)
H15	0.7594	0.2907	0.2721	0.033*

C16	0.5994 (2)	0.24347 (11)	0.3291 (2)	0.0228 (4)
H16	0.6550	0.2103	0.3913	0.027*
C17	0.29536 (19)	0.11402 (10)	0.26658 (19)	0.0187 (4)
C18	0.3096 (2)	0.04341 (11)	0.3035 (2)	0.0247 (4)
H18	0.3610	0.0302	0.3949	0.030*
C19	0.2487 (2)	−0.00782 (12)	0.2068 (2)	0.0289 (5)
H19	0.2576	−0.0560	0.2323	0.035*
C20	0.1746 (2)	0.01165 (12)	0.0725 (2)	0.0280 (5)
H20	0.1337	−0.0234	0.0062	0.034*
C21	0.1601 (2)	0.08144 (13)	0.0353 (2)	0.0280 (4)
H21	0.1089	0.0943	−0.0565	0.034*
C22	0.2201 (2)	0.13322 (11)	0.1311 (2)	0.0234 (4)
H22	0.2102	0.1813	0.1050	0.028*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.02718 (12)	0.02680 (13)	0.01673 (11)	0.00020 (8)	−0.00029 (8)	0.00236 (8)
P1	0.0171 (2)	0.0201 (2)	0.0142 (2)	−0.00042 (17)	0.00361 (17)	−0.00038 (18)
O1	0.0194 (6)	0.0253 (7)	0.0178 (6)	−0.0003 (5)	0.0063 (5)	−0.0041 (5)
C1	0.0204 (9)	0.0220 (10)	0.0176 (9)	0.0006 (7)	0.0095 (7)	0.0010 (7)
C2	0.0190 (9)	0.0294 (11)	0.0210 (9)	0.0005 (7)	0.0067 (7)	0.0026 (8)
C3	0.0203 (9)	0.0304 (11)	0.0294 (11)	0.0044 (8)	0.0114 (8)	0.0054 (9)
C4	0.0276 (10)	0.0212 (10)	0.0251 (10)	0.0024 (8)	0.0151 (8)	0.0040 (8)
C5	0.0359 (11)	0.0261 (11)	0.0384 (12)	0.0028 (9)	0.0235 (10)	0.0002 (9)
C6	0.0506 (14)	0.0265 (12)	0.0368 (12)	−0.0002 (10)	0.0262 (11)	−0.0065 (10)
C7	0.0447 (13)	0.0290 (12)	0.0242 (10)	−0.0051 (10)	0.0122 (10)	−0.0060 (9)
C8	0.0312 (10)	0.0253 (11)	0.0208 (9)	−0.0008 (8)	0.0098 (8)	−0.0003 (8)
C9	0.0257 (9)	0.0215 (10)	0.0184 (9)	−0.0006 (7)	0.0112 (8)	0.0018 (7)
C10	0.0195 (8)	0.0230 (10)	0.0181 (9)	0.0016 (7)	0.0077 (7)	0.0012 (7)
C11	0.0187 (8)	0.0210 (9)	0.0160 (8)	−0.0017 (7)	0.0051 (7)	−0.0042 (7)
C12	0.0235 (9)	0.0219 (10)	0.0216 (9)	0.0006 (7)	0.0081 (8)	−0.0010 (8)
C13	0.0377 (12)	0.0222 (10)	0.0255 (10)	−0.0001 (8)	0.0132 (9)	−0.0004 (8)
C14	0.0399 (12)	0.0260 (11)	0.0293 (11)	−0.0105 (9)	0.0218 (10)	−0.0076 (9)
C15	0.0233 (9)	0.0342 (12)	0.0305 (11)	−0.0087 (8)	0.0148 (9)	−0.0133 (9)
C16	0.0196 (9)	0.0269 (10)	0.0221 (9)	−0.0004 (7)	0.0061 (7)	−0.0085 (8)
C17	0.0178 (8)	0.0220 (10)	0.0170 (8)	−0.0035 (7)	0.0062 (7)	−0.0036 (7)
C18	0.0218 (9)	0.0254 (11)	0.0250 (10)	0.0005 (8)	0.0032 (8)	0.0008 (8)
C19	0.0259 (10)	0.0216 (10)	0.0377 (12)	−0.0002 (8)	0.0059 (9)	−0.0041 (9)
C20	0.0226 (9)	0.0332 (12)	0.0292 (11)	−0.0048 (8)	0.0088 (8)	−0.0133 (9)
C21	0.0281 (10)	0.0387 (13)	0.0174 (9)	−0.0084 (9)	0.0069 (8)	−0.0045 (9)
C22	0.0263 (10)	0.0254 (11)	0.0182 (9)	−0.0044 (8)	0.0053 (8)	0.0015 (8)

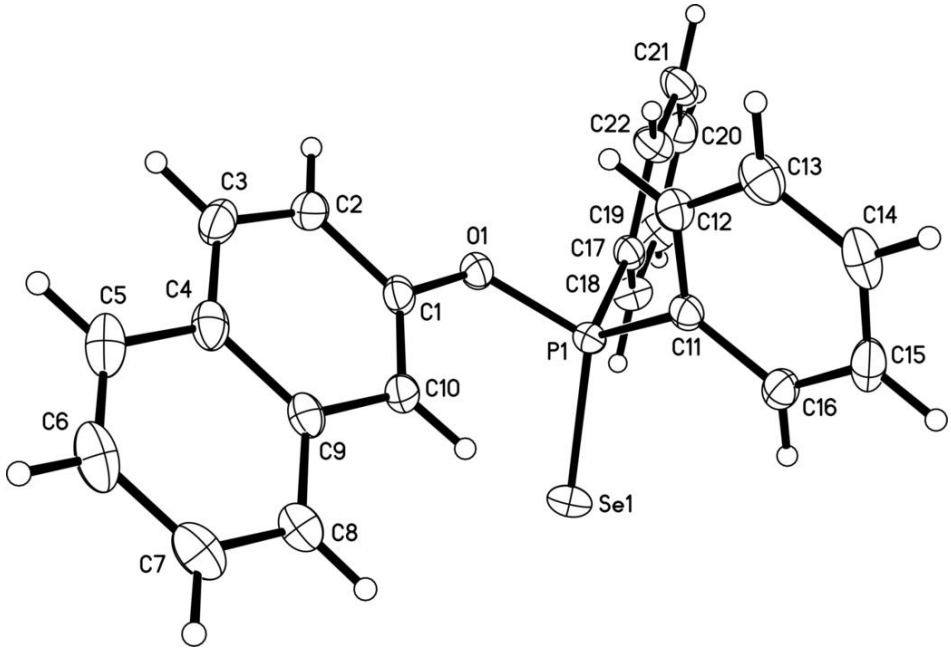
Geometric parameters (Å, °)

Se1—P1	2.0890 (5)	C11—C12	1.398 (3)
P1—O1	1.6200 (14)	C11—C16	1.401 (3)
P1—C17	1.805 (2)	C12—C13	1.395 (3)
P1—C11	1.808 (2)	C12—H12	0.9500

O1—C1	1.400 (2)	C13—C14	1.387 (3)
C1—C10	1.362 (3)	C13—H13	0.9500
C1—C2	1.416 (3)	C14—C15	1.385 (3)
C2—C3	1.361 (3)	C14—H14	0.9500
C2—H2	0.9500	C15—C16	1.393 (3)
C3—C4	1.420 (3)	C15—H15	0.9500
C3—H3	0.9500	C16—H16	0.9500
C4—C5	1.420 (3)	C17—C18	1.391 (3)
C4—C9	1.424 (3)	C17—C22	1.403 (3)
C5—C6	1.367 (4)	C18—C19	1.390 (3)
C5—H5	0.9500	C18—H18	0.9500
C6—C7	1.409 (3)	C19—C20	1.391 (3)
C6—H6	0.9500	C19—H19	0.9500
C7—C8	1.371 (3)	C20—C21	1.377 (3)
C7—H7	0.9500	C20—H20	0.9500
C8—C9	1.417 (3)	C21—C22	1.390 (3)
C8—H8	0.9500	C21—H21	0.9500
C9—C10	1.424 (3)	C22—H22	0.9500
C10—H10	0.9500		
O1—P1—C17	97.68 (8)	C12—C11—C16	119.78 (18)
O1—P1—C11	103.29 (8)	C12—C11—P1	119.85 (14)
C17—P1—C11	108.10 (9)	C16—C11—P1	120.32 (15)
O1—P1—Se1	116.37 (5)	C13—C12—C11	120.33 (19)
C17—P1—Se1	114.05 (7)	C13—C12—H12	119.8
C11—P1—Se1	115.41 (6)	C11—C12—H12	119.8
C1—O1—P1	126.43 (12)	C14—C13—C12	119.6 (2)
C10—C1—O1	125.14 (17)	C14—C13—H13	120.2
C10—C1—C2	121.84 (18)	C12—C13—H13	120.2
O1—C1—C2	113.00 (17)	C15—C14—C13	120.3 (2)
C3—C2—C1	119.76 (19)	C15—C14—H14	119.8
C3—C2—H2	120.1	C13—C14—H14	119.8
C1—C2—H2	120.1	C14—C15—C16	120.77 (19)
C2—C3—C4	120.74 (19)	C14—C15—H15	119.6
C2—C3—H3	119.6	C16—C15—H15	119.6
C4—C3—H3	119.6	C15—C16—C11	119.2 (2)
C5—C4—C3	122.15 (19)	C15—C16—H16	120.4
C5—C4—C9	118.9 (2)	C11—C16—H16	120.4
C3—C4—C9	118.93 (18)	C18—C17—C22	119.71 (18)
C6—C5—C4	120.7 (2)	C18—C17—P1	120.56 (15)
C6—C5—H5	119.6	C22—C17—P1	119.72 (15)
C4—C5—H5	119.6	C19—C18—C17	120.10 (19)
C5—C6—C7	120.3 (2)	C19—C18—H18	120.0
C5—C6—H6	119.9	C17—C18—H18	119.9
C7—C6—H6	119.9	C18—C19—C20	119.8 (2)
C8—C7—C6	120.7 (2)	C18—C19—H19	120.1
C8—C7—H7	119.7	C20—C19—H19	120.1
C6—C7—H7	119.7	C21—C20—C19	120.4 (2)
C7—C8—C9	120.5 (2)	C21—C20—H20	119.8
C7—C8—H8	119.8	C19—C20—H20	119.8

C9—C8—H8	119.8	C20—C21—C22	120.4 (2)
C8—C9—C10	121.63 (18)	C20—C21—H21	119.8
C8—C9—C4	118.96 (19)	C22—C21—H21	119.8
C10—C9—C4	119.40 (18)	C21—C22—C17	119.6 (2)
C1—C10—C9	119.29 (18)	C21—C22—H22	120.2
C1—C10—H10	120.4	C17—C22—H22	120.2
C9—C10—H10	120.4		

Fig. 1


C21
C22
C20
C13
C3
C2
C19
C12
C14
O1
C17
C18
C5
C4
C1
P1
C11
C15
C10
C16
C6
C9
Se1
C8
C7