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Crystal structures of bis[2-(diphenylphosphinothioyl)phenyl] ether and bis{2-[diphenyl(selanylidene)phosphanyl]phenyl} ether

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The title compounds, $C_{36}H_{28}OP_2S_2$, (1), and $C_{36}H_{28}OP_2Se_2$, (2), exhibit remarkably similar structures although they are not isomorphous. The whole molecule of compound (2) is generated by twofold symmetry, with the ether O atom located on the twofold axis. Both compounds have intramolecular π–π interactions between terminal phenyl rings with centroid–centroid distances of 3.6214 (16) and 3.8027 (14) Å in (1) and (2), respectively. In the crystal of (1), short C—H$\cdots$S hydrogen bonds link the molecules, forming chains along [001], while in (2) there are no analogous C—H$\cdots$Se interactions present.

1. Chemical context

The ligand bis[2-(diphenylphosphanyl)phenyl] ether (POP) and its congeners, including the more rigid Xantphos [(9,9-dimethyl-9H-xanthene-4,5-diyl)bis(diphenylphosphane)], comprise a series of chelating diphosphines with a range of flexibility to accommodate variable 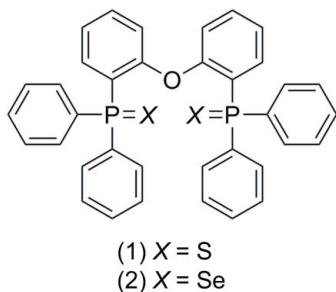bonding geometries at transition metals. Experimental and theoretical studies of metal complexes with diphosphines have shown a strong correlation between diphosphine bite angle and selectivity in catalytic transformations (Dierkes & van Leeuwen, 1999; Gathy et al., 2011). Simple functionalization of these diphosphines to form diphosphine dioxides, disulfides, and diselenides has permitted further tuning of the bonding of these ligands to metals by changing the bite-angle range as well as the electronic properties of these ligands. The π-accepting phosphorous donor atoms of the parent diphosphines are profoundly altered with the addition of π-donor chalcogen donor atoms (Dairiki et al., 2009). Chalcogen-modified diphosphine ligands have been utilized in strategies to tune the catalytic behavior of systems including the Pd[II]-catalysed hydroamination of dienes (Jahromi et al., 2012) and Ru[II] transfer hydrogenation of aldehydes and ketones (Deb et al., 2010). Hemilability, implicated in the selectivity and reactivity of some catalytic reactions (Braunstein et al., 2001), can also result from the chalcogen functionalization of phosphines as well (Deb et al., 2010).

Our interest in the application of chalcogen-substituted diphosphines to alter the electronic features of photoluminescent Cu[I] sensor materials (Smith et al., 2010) led us to study the solid-state structural features of the dichalcogen diphosphines, including the disulfide and diselenide of the ligand POP. We wanted to investigate the inter- and intramolecular features that dominate the solid-state structural behavior of these ligands. The molecular geometry and

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packing of these chalcogen diphosphines may strongly influence the geometric features of their d^{10} metal complexes, as d^{10} metals typically have poor stereochemical preferences. In this study, the structures obtained for bis[2-(diphenylphosphinothioyl)phenyl] ether, (1), and bis{2-[diphenyl-(selanylidene)phosphanyl]phenyl} ether, (2), are compared.

(1) X = S
(2) X = Se

2. Structural commentary

The molecular structures of (1) and (2) are illustrated in Figs. 1 and 2, respectively. The P—S [1.9543 (8) and 1.9552 (9) Å] and P—Se [2.1125 (6) Å] bond lengths are consistent with covalent
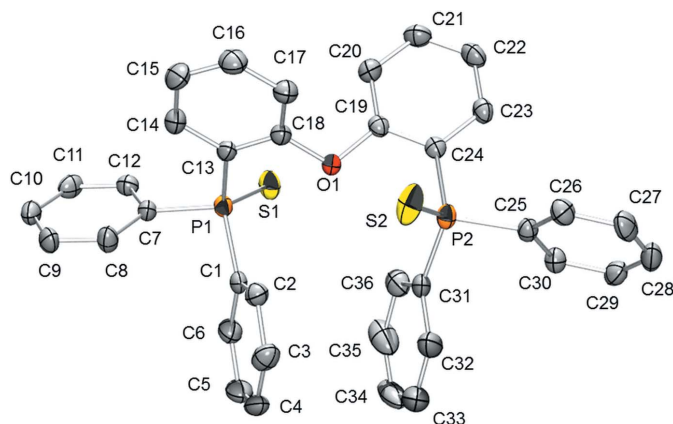

Figure 1
The molecular structure of (1), showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.
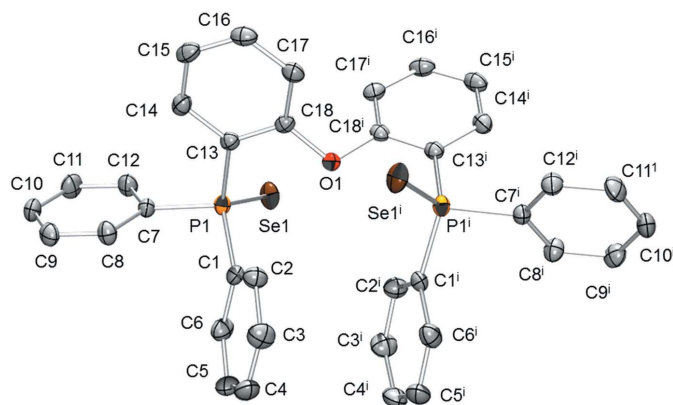

Figure 2
The molecular structure of (2), showing the atom labelling and displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (i) $-x, y, -z + \frac{3}{2}$.]
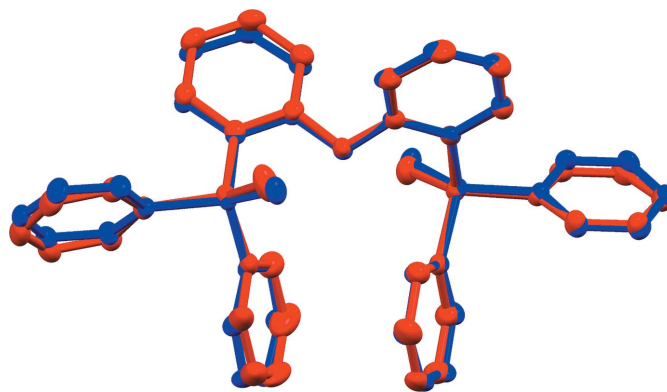

Figure 3
Structural overlay of (1) (red) and (2) (blue).

radii predictions as well as typical bond lengths for diarylphosphine sulfides and selenides. Although these structures are not isomorphous, many intramolecular features are remarkably alike despite the potentially flexible ether linkage of the diphosphine backbone. To demonstrate the similarity, several metrics were compared. The intramolecular P···P distances [5.6452 (8) Å for (1); 5.669 (1) Å for (2)], the intramolecular E···E distances [E = S 6.636 (1) Å for (1); E = Se 6.8246 (7) Å for (2)], and the EP···PE angles [158.29 (4)° for (1); 158.44 (2)° for (2)] all indicate a common geometry near the phosphorous–chalcogen bonds. This similarity extends to the phenyl ring orientations. A structural overlap calculation of the pairwise atomic coordinates of all related atoms of (1) and (2) (except the chalcogens) reveals an r.m.s. deviation of only 0.214 Å over 39 atom pairs (Fig. 3).

The largest differences in the intramolecular features of (1) and (2) can be found in the closest approach of a pair of terminal phenyl rings, each bonded to different phosphorous atoms (Fig. 4). In the structure of (2), the angle between mean planes formed by atoms C1–C6 and the twofold axis-related atoms C1–C6 of the same molecule is 0.98 (12)°, with a centroid–centroid distance of 3.8027 (14) Å. The analogous relationship in the structure of (1), involving phenyl rings C1–C6 and C31–C36, is a dihedral angle of 6.52 (13)° and a
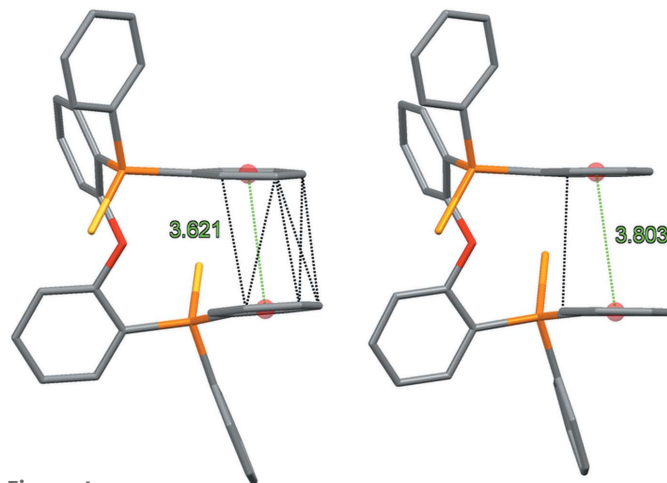

Figure 4
Intramolecular π–π interactions in (1) and (2).

Table 1
Hydrogen-bond geometry (Å, °) for (1).

Cg4 is the centroid of ring C19–C24.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C11—H11$\cdots$S2$^{\text{i}}$	0.95	2.82	3.696 (2)	153
C4—H4$\cdots$S2$^{\text{ii}}$	0.95	2.94	3.698 (3)	138
C5—H5$\cdots$S1$^{\text{iii}}$	0.95	2.93	3.796 (3)	152
C9—H9$\cdots$Cg4$^{\text{iv}}$	0.95	2.94	3.598 (3)	127

Symmetry codes: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (iii) $x-\frac{1}{2}, y, -z+\frac{1}{2}$; (iv) $-x+\frac{3}{2}, y-\frac{1}{2}, z$.

Table 2
Hydrogen-bond geometry (Å, °) for (2).

Cg2 and Cg3 are the centroids of rings C7–C12 and C13–C18, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C5—H5$\cdots$Cg2$^{\text{i}}$	0.95	2.63	3.546 (3)	161
C9—H9$\cdots$Cg3$^{\text{ii}}$	0.95	2.94	3.676 (3)	135

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$.

centroid–centroid distance of 3.6214 (16) Å. The result of these differences is that in (2) there is only one C$\cdots$C intra-molecular contact between these phenyl rings shorter than 3.6 Å, while in (1) there are six unique contacts that meet this criteria. Although these intramolecular C$\cdots$C contacts are slightly longer than the van der Waals radii sum of 3.4 Å, the additional C$\cdots$C close-contacts in (1) may contribute to stronger intramolecular π–π interactions between these phenyl rings compared to (2). The dihedral angles between the mean planes formed by the ether-linked phenyl groups [(C13–C18 and C19–C24) 76.83 (11)° for (1); (C13–C18 and the symmetry-related C13–C18 ring) 84.53 (11)° for (2)] also show a significant difference in the twist around the ether linkage.

Figure 6
Crystal packing of (1), viewed along [010] (above) and [100] (below). Color to highlight molecules packing within columns.
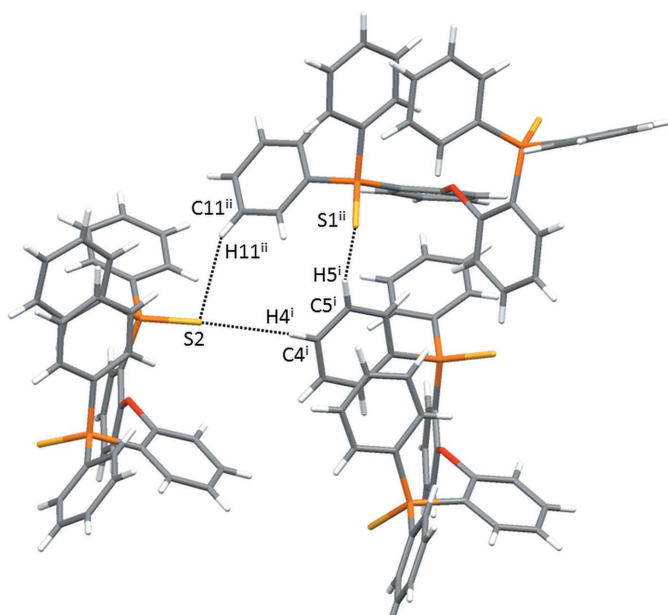

Figure 5
Intermolecular C—H$\cdots$S interactions in (1). [Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.]
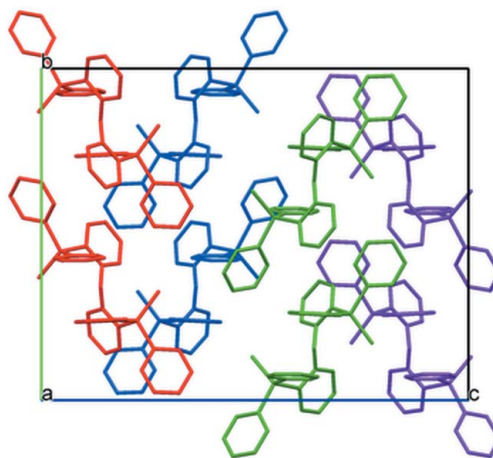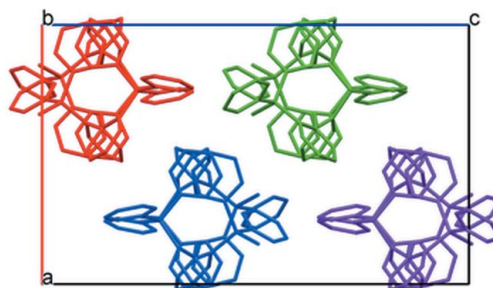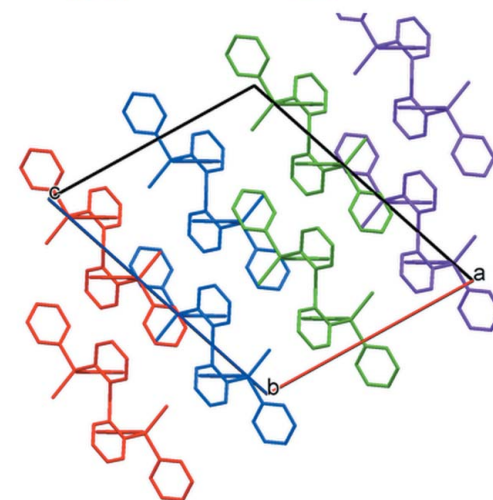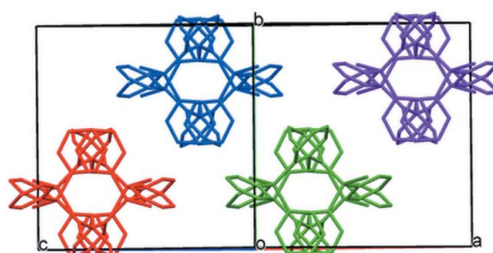

Figure 7
Crystal packing of (2) viewed along [101] (above) and [010] (below). Color to highlight molecules packing within columns.

Table 3
Experimental details.

	(1)	(2)
Crystal data		
Chemical formula	$C_{36}H_{28}OP_2S_2$	$C_{36}H_{28}OP_2Se_2$
M_r	602.64	696.44
Crystal system, space group	Orthorhombic, $Pbca$	Monoclinic, $C2/c$
Temperature (K)	173	173
a, b, c (Å)	14.1161 (9), 18.0874 (12), 23.1986 (16)	14.0964 (15), 13.0854 (13), 17.5918 (18)
α, β, γ (°)	90, 90, 90	90, 109.226 (8), 90
V (Å^3)	5923.1 (7)	3064.0 (6)
Z	8	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.32	2.55
Crystal size (mm)	$0.52 \times 0.24 \times 0.12$	$0.80 \times 0.12 \times 0.12$
Data collection		
Diffractometer	Rigaku XtaLAB mini	Rigaku XtaLAB mini
Absorption correction	Multi-scan (*REQAB*; Rigaku, 1998)	Multi-scan (*REQAB;* Rigaku, 1998)
T_{min}, T_{max}	0.718, 0.963	0.556, 0.737
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	54343, 6050, 4671	15840, 3521, 2958
R_{int}	0.073	0.045
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.649
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.101, 1.07	0.032, 0.066, 1.07
No. of reflections	6050	3521
No. of parameters	370	186
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.37, −0.33	0.40, −0.41

Computer programs: *CrystalClear-SM Expert* (Rigaku Americas and Rigaku, 2011), *SIR2004* (Burla *et al.*, 2005), *SHELXL2013* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *CrystalStructure* (Rigaku, 2010).

3. Supramolecular features

The intermolecular features of (1) and (2) reveal additional differences between these seemingly similar structures. In the crystal of (1), most notably there are three unique intermolecular C—H···S interactions (Table 1) shorter than the sum of the van der Waals radii. Each molecule participates as a C—H donor with two different S2 acceptors as well as one S1 acceptor (Table 1 and Fig. 5). As such, each molecule is involved in C—H···S intermolecular interactions with three other unique molecules. In the crystal of (2), no analogous C—H···Se intermolecular interactions are present.

Both structures show that several intermolecular C—H···π contacts less than *ca* 3.0 Å are present but these are likely to play a weak role in packing interactions [see Table 1 for (1) and Table 2 for (2)]. Molecules of (1) stack in columns parallel to [010] (Fig. 6). The intramolecular π–π stacking interactions of (1) are all aligned perpendicular to the column stacking axis. Molecules of (2) stack in columns parallel to [101] (Fig. 7) with intramolecular π–π stacking perpendicular to the column stacking vector.

4. Database survey

The Cambridge Structural Database (Version 5.35; Groom & Allen, 2014) contains several closely related phosphine sulfide structures, including Xantphos disulfide (Jahromi *et al.*, 2012), POP monosulfide (Deb *et al.*, 2010), and POP dioxide (Deb & Dutta, 2010). As the xanthene backbone of the diphosphine linkage is more sterically constrained compared with the ether linkage of POP, the Xantphos disulfide structure forces the intramolecular S···S [4.207 (1) Å] and P···P [4.984 (1) Å] distances to be much shorter compared with (1). The structure of POP monosulfide is also very different from (1), as intramolecular phenyl ring interactions are present but these involve a terminal phenyl ring and a bridging phenyl ring rather than two terminal phenyl rings as in (1). POP dioxide adopts a conformation unlike (1) or (2), as the P—O bond vectors are closer to antiparallel [intramolecular OP···P—O angles of 37.0 (6)°]. Considering metal complexes of related ligands, the structures of only two ruthenium(II) complexes (Deb *et al.*, 2010), three palladium(II) complexes (Milheiro & Faller, 2011; Saikia *et al.*, 2012), and one rhodium(I) complex (Faller *et al.*, 2008) have been reported with Xantphos sulfide or POP sulfide. The structure of only one palladium(II) complex of Xantphos disulfide (Jahromi *et al.*, 2012) is reported. POP or Xantphos selenide structures are even rarer, as only one copper(I) complex of POP selenide is reported (Venkateswaran *et al.*, 2007b). No structures to date have been reported with diselenides of POP or Xantphos.

5. Synthesis and crystallization

Compounds (1) and (2) were prepared using a reported procedure (Venkateswaran *et al.*, 2007a). Crystals of each sample were obtained by diffusion of diethyl ether into a concentrated dichloromethane solution.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were placed in calculated positions and refined in the riding-model approximation: C—H = 0.95 Å with $U_{iso}(H) = 1.2U_{eq}(C)$.

A small number of low-angle reflections [nine for (1) and five for (2)] were missing from these high-quality data sets due to the arrangement of the instrument with a conservatively sized beam stop and a fixed-position detector. The large number of reflections in the data sets (and the Fourier-transform relationship of intensities to atoms) ensures that no particular bias was thereby introduced into this routine structure determination.

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supporting information

Crystal structures of bis[2-(diphenylphosphinothioyl)phenyl] ether and bis{2-[diphenyl(selanylidene)phosphanyl]phenyl} ether

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Computing details

For both compounds, data collection: *CrystalClear-SM Expert* (Rigaku Americas and Rigaku, 2011); cell refinement: *CrystalClear-SM Expert* (Rigaku Americas and Rigaku, 2011); data reduction: *CrystalClear-SM Expert* (Rigaku Americas and Rigaku, 2011); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2010).

(1) {2-[2-(Diphenylphosphinothioyl)phenoxy]phenyl}diphenylphosphanethione

Crystal data

$C_{36}H_{28}OP_2S_2$	$D_x = 1.352$ Mg m^{-3}
$M_r = 602.64$	Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Orthorhombic, *Pbca*	Cell parameters from 42656 reflections
$a = 14.1161$ (9) Å	$\theta = 3.0–26.5°$
$b = 18.0874$ (12) Å	$\mu = 0.32$ mm^{-1}
$c = 23.1986$ (16) Å	$T = 173$ K
$V = 5923.1$ (7) Å^3	Prism, colorless
$Z = 8$	$0.52 \times 0.24 \times 0.12$ mm
$F(000) = 2512$	

Data collection

Rigaku XtaLAB mini diffractometer	54343 measured reflections
Radiation source: normal-focu sealed tube	6050 independent reflections
Detector resolution: 6.849 pixels mm^{-1}	4671 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.073$
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)	$\theta_{max} = 26.4°$, $\theta_{min} = 3.1°$
	$h = -17 \rightarrow 17$
	$k = -22 \rightarrow 22$
$T_{min} = 0.718$, $T_{max} = 0.963$	$l = -28 \rightarrow 28$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.101$	$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2 + 4.2594P]$
$S = 1.07$	where $P = (F_o^2 + 2F_c^2)/3$
6050 reflections	$(\Delta/\sigma)_{max} = 0.001$
370 parameters	$\Delta\rho_{max} = 0.37$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.33$ e Å^{-3}

Special details

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.76118 (5)	0.32675 (3)	0.22627 (3)	0.03418 (16)
S2	0.84441 (6)	0.36984 (4)	0.50579 (3)	0.0443 (2)
P1	0.75393 (4)	0.24001 (3)	0.27630 (2)	0.02270 (14)
P2	0.79892 (4)	0.44866 (3)	0.45519 (2)	0.02408 (14)
O1	0.84740 (10)	0.34242 (8)	0.36159 (6)	0.0249 (3)
C1	0.65450 (15)	0.24111 (11)	0.32542 (9)	0.0237 (5)
C2	0.66367 (17)	0.23755 (13)	0.38463 (10)	0.0290 (5)
H2	0.7248	0.2363	0.4017	0.035*
C3	0.58330 (18)	0.23575 (14)	0.41906 (11)	0.0384 (6)
H3	0.5895	0.2330	0.4598	0.046*
C4	0.49506 (18)	0.23795 (14)	0.39448 (13)	0.0408 (7)
H4	0.4402	0.2364	0.4182	0.049*
C5	0.48573 (18)	0.24238 (15)	0.33517 (13)	0.0421 (7)
H5	0.4245	0.2446	0.3183	0.051*
C6	0.56461 (17)	0.24356 (14)	0.30074 (11)	0.0343 (6)
H6	0.5580	0.2461	0.2600	0.041*
C7	0.73603 (15)	0.15479 (11)	0.23648 (9)	0.0229 (5)
C8	0.70755 (18)	0.09086 (12)	0.26540 (10)	0.0311 (5)
H8	0.6945	0.0928	0.3055	0.037*
C9	0.69823 (17)	0.02464 (13)	0.23609 (11)	0.0328 (6)
H9	0.6791	−0.0187	0.2560	0.039*
C10	0.71694 (17)	0.02185 (13)	0.17759 (11)	0.0329 (6)
H10	0.7119	−0.0237	0.1575	0.039*
C11	0.74291 (17)	0.08518 (14)	0.14842 (10)	0.0324 (6)
H11	0.7543	0.0833	0.1081	0.039*
C12	0.75247 (15)	0.15149 (13)	0.17768 (9)	0.0264 (5)
H12	0.7704	0.1949	0.1573	0.032*
C13	0.85929 (15)	0.22209 (12)	0.31969 (9)	0.0240 (5)
C14	0.90793 (17)	0.15465 (13)	0.31680 (11)	0.0330 (6)
H14	0.8853	0.1170	0.2918	0.040*
C15	0.98812 (18)	0.14166 (14)	0.34947 (12)	0.0405 (6)
H15	1.0208	0.0960	0.3462	0.049*
C16	1.02045 (18)	0.19535 (14)	0.38683 (12)	0.0378 (6)
H16	1.0750	0.1862	0.4097	0.045*
C17	0.97394 (16)	0.26249 (13)	0.39116 (11)	0.0318 (5)
H17	0.9955	0.2991	0.4174	0.038*
C18	0.89568 (15)	0.27550 (12)	0.35685 (10)	0.0249 (5)
C19	0.90192 (15)	0.40629 (12)	0.35800 (9)	0.0239 (5)
C20	0.97288 (16)	0.41302 (13)	0.31744 (10)	0.0299 (5)

H20	0.9869	0.3733	0.2921	0.036*
C21	1.02346 (17)	0.47847 (14)	0.31416 (11)	0.0342 (6)
H21	1.0731	0.4833	0.2868	0.041*
C22	1.00247 (17)	0.53676 (13)	0.35025 (10)	0.0332 (6)
H22	1.0370	0.5817	0.3474	0.040*
C23	0.93094 (16)	0.52955 (12)	0.39068 (10)	0.0273 (5)
H23	0.9166	0.5698	0.4155	0.033*
C24	0.87957 (15)	0.46395 (12)	0.39544 (9)	0.0225 (5)
C25	0.78799 (16)	0.53749 (12)	0.49171 (9)	0.0249 (5)
C26	0.83608 (17)	0.54978 (13)	0.54298 (10)	0.0313 (5)
H26	0.8779	0.5132	0.5577	0.038*
C27	0.82286 (19)	0.61579 (14)	0.57274 (11)	0.0372 (6)
H27	0.8555	0.6241	0.6080	0.045*
C28	0.76293 (19)	0.66911 (14)	0.55147 (11)	0.0373 (6)
H28	0.7542	0.7140	0.5721	0.045*
C29	0.71556 (17)	0.65764 (13)	0.50035 (11)	0.0335 (6)
H29	0.6747	0.6948	0.4856	0.040*
C30	0.72726 (16)	0.59212 (12)	0.47047 (10)	0.0278 (5)
H30	0.6939	0.5842	0.4354	0.033*
C31	0.68058 (16)	0.43557 (12)	0.42751 (11)	0.0295 (5)
C32	0.6092 (2)	0.42773 (16)	0.46861 (14)	0.0516 (8)
H32	0.6250	0.4267	0.5084	0.062*
C33	0.5165 (2)	0.42145 (18)	0.4520 (2)	0.0707 (11)
H33	0.4682	0.4167	0.4803	0.085*
C34	0.4934 (2)	0.42201 (17)	0.3948 (2)	0.0689 (11)
H34	0.4290	0.4175	0.3835	0.083*
C35	0.5633 (2)	0.42916 (16)	0.35337 (16)	0.0577 (9)
H35	0.5468	0.4293	0.3137	0.069*
C36	0.65762 (18)	0.43611 (14)	0.36972 (12)	0.0370 (6)
H36	0.7058	0.4412	0.3414	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0458 (4)	0.0225 (3)	0.0343 (3)	−0.0026 (3)	0.0019 (3)	0.0067 (3)
S2	0.0743 (5)	0.0295 (3)	0.0289 (3)	0.0155 (3)	0.0029 (3)	0.0074 (3)
P1	0.0250 (3)	0.0189 (3)	0.0241 (3)	−0.0008 (2)	0.0017 (2)	0.0006 (2)
P2	0.0300 (3)	0.0201 (3)	0.0221 (3)	0.0005 (2)	0.0013 (2)	0.0002 (2)
O1	0.0214 (8)	0.0210 (8)	0.0324 (9)	−0.0002 (6)	0.0013 (7)	−0.0049 (7)
C1	0.0243 (12)	0.0169 (10)	0.0299 (12)	−0.0011 (9)	0.0011 (9)	−0.0018 (9)
C2	0.0270 (12)	0.0283 (12)	0.0318 (13)	0.0015 (10)	0.0024 (10)	0.0020 (10)
C3	0.0417 (16)	0.0390 (15)	0.0346 (14)	0.0041 (12)	0.0127 (12)	0.0047 (12)
C4	0.0286 (14)	0.0297 (14)	0.0642 (19)	−0.0001 (11)	0.0197 (13)	0.0014 (13)
C5	0.0236 (13)	0.0405 (15)	0.0622 (19)	−0.0006 (11)	−0.0018 (13)	−0.0022 (14)
C6	0.0291 (13)	0.0339 (14)	0.0397 (14)	−0.0012 (11)	−0.0042 (11)	−0.0025 (11)
C7	0.0227 (11)	0.0204 (11)	0.0256 (11)	−0.0002 (9)	0.0022 (9)	−0.0014 (9)
C8	0.0408 (14)	0.0251 (12)	0.0274 (12)	−0.0038 (11)	0.0078 (11)	−0.0005 (10)
C9	0.0369 (14)	0.0209 (11)	0.0407 (14)	−0.0029 (10)	0.0076 (12)	0.0015 (10)

C10	0.0289 (13)	0.0286 (13)	0.0413 (14)	0.0003 (10)	−0.0016 (11)	−0.0106 (11)
C11	0.0305 (13)	0.0426 (14)	0.0239 (12)	0.0026 (11)	0.0009 (10)	−0.0071 (11)
C12	0.0236 (12)	0.0284 (12)	0.0271 (12)	−0.0010 (10)	0.0012 (10)	0.0027 (10)
C13	0.0219 (11)	0.0205 (11)	0.0296 (12)	−0.0003 (9)	0.0056 (9)	0.0012 (9)
C14	0.0304 (13)	0.0250 (12)	0.0435 (15)	0.0005 (10)	0.0017 (11)	−0.0034 (11)
C15	0.0319 (14)	0.0290 (13)	0.0607 (18)	0.0088 (11)	0.0005 (13)	0.0020 (13)
C16	0.0262 (13)	0.0383 (15)	0.0487 (16)	0.0028 (11)	−0.0046 (12)	0.0046 (12)
C17	0.0250 (12)	0.0323 (13)	0.0383 (14)	−0.0007 (10)	−0.0007 (11)	−0.0007 (11)
C18	0.0226 (12)	0.0233 (11)	0.0288 (12)	−0.0006 (9)	0.0047 (9)	0.0002 (9)
C19	0.0213 (12)	0.0239 (11)	0.0266 (12)	−0.0005 (9)	−0.0045 (9)	0.0006 (9)
C20	0.0270 (13)	0.0309 (13)	0.0316 (13)	0.0017 (10)	0.0020 (10)	−0.0014 (10)
C21	0.0269 (13)	0.0390 (14)	0.0366 (14)	−0.0027 (11)	0.0060 (11)	0.0072 (11)
C22	0.0301 (13)	0.0279 (13)	0.0416 (14)	−0.0066 (10)	−0.0021 (11)	0.0074 (11)
C23	0.0293 (13)	0.0214 (11)	0.0312 (13)	0.0002 (10)	−0.0042 (10)	0.0009 (10)
C24	0.0216 (11)	0.0228 (11)	0.0232 (11)	0.0017 (9)	−0.0042 (9)	0.0021 (9)
C25	0.0291 (12)	0.0229 (11)	0.0226 (11)	−0.0016 (9)	0.0034 (9)	−0.0010 (9)
C26	0.0322 (13)	0.0318 (13)	0.0298 (13)	−0.0022 (11)	−0.0026 (10)	0.0005 (11)
C27	0.0426 (16)	0.0408 (15)	0.0282 (13)	−0.0115 (12)	−0.0012 (11)	−0.0093 (11)
C28	0.0445 (15)	0.0279 (13)	0.0396 (14)	−0.0059 (11)	0.0110 (12)	−0.0092 (11)
C29	0.0333 (14)	0.0263 (12)	0.0409 (15)	0.0034 (10)	0.0088 (11)	−0.0006 (11)
C30	0.0311 (13)	0.0258 (12)	0.0263 (12)	−0.0004 (10)	−0.0005 (10)	−0.0010 (10)
C31	0.0276 (13)	0.0218 (12)	0.0392 (14)	−0.0021 (9)	0.0054 (11)	−0.0083 (10)
C32	0.0435 (18)	0.0489 (17)	0.0623 (19)	−0.0169 (14)	0.0226 (15)	−0.0221 (15)
C33	0.0399 (19)	0.052 (2)	0.121 (3)	−0.0127 (15)	0.029 (2)	−0.032 (2)
C34	0.0216 (16)	0.0352 (17)	0.150 (4)	−0.0002 (12)	−0.012 (2)	−0.004 (2)
C35	0.0474 (19)	0.0404 (17)	0.085 (2)	−0.0005 (14)	−0.0300 (18)	0.0086 (16)
C36	0.0334 (14)	0.0304 (13)	0.0472 (16)	0.0017 (11)	−0.0065 (12)	0.0039 (12)

Geometric parameters (Å, º)

S1—P1	1.9543 (8)	C15—H15	0.9500
S2—P2	1.9552 (8)	C16—C17	1.384 (3)
P1—C1	1.808 (2)	C16—H16	0.9500
P1—C7	1.815 (2)	C17—C18	1.382 (3)
P1—C13	1.825 (2)	C17—H17	0.9500
P2—C31	1.805 (2)	C19—C20	1.380 (3)
P2—C24	1.815 (2)	C19—C24	1.393 (3)
P2—C25	1.823 (2)	C20—C21	1.384 (3)
O1—C19	1.391 (3)	C20—H20	0.9500
O1—C18	1.393 (3)	C21—C22	1.378 (3)
C1—C2	1.381 (3)	C21—H21	0.9500
C1—C6	1.393 (3)	C22—C23	1.384 (3)
C2—C3	1.388 (3)	C22—H22	0.9500
C2—H2	0.9500	C23—C24	1.395 (3)
C3—C4	1.370 (4)	C23—H23	0.9500
C3—H3	0.9500	C25—C26	1.387 (3)
C4—C5	1.385 (4)	C25—C30	1.398 (3)
C4—H4	0.9500	C26—C27	1.392 (3)

C5—C6	1.370 (3)	C26—H26	0.9500
C5—H5	0.9500	C27—C28	1.374 (4)
C6—H6	0.9500	C27—H27	0.9500
C7—C12	1.385 (3)	C28—C29	1.377 (4)
C7—C8	1.396 (3)	C28—H28	0.9500
C8—C9	1.384 (3)	C29—C30	1.383 (3)
C8—H8	0.9500	C29—H29	0.9500
C9—C10	1.383 (3)	C30—H30	0.9500
C9—H9	0.9500	C31—C36	1.379 (3)
C10—C11	1.380 (3)	C31—C32	1.395 (3)
C10—H10	0.9500	C32—C33	1.368 (5)
C11—C12	1.385 (3)	C32—H32	0.9500
C11—H11	0.9500	C33—C34	1.366 (5)
C12—H12	0.9500	C33—H33	0.9500
C13—C18	1.393 (3)	C34—C35	1.384 (5)
C13—C14	1.401 (3)	C34—H34	0.9500
C14—C15	1.382 (3)	C35—C36	1.390 (4)
C14—H14	0.9500	C35—H35	0.9500
C15—C16	1.379 (4)	C36—H36	0.9500
C1—P1—C7	102.84 (10)	C18—C17—C16	119.1 (2)
C1—P1—C13	106.68 (10)	C18—C17—H17	120.4
C7—P1—C13	104.09 (10)	C16—C17—H17	120.4
C1—P1—S1	113.96 (8)	C17—C18—C13	122.2 (2)
C7—P1—S1	112.76 (7)	C17—C18—O1	119.6 (2)
C13—P1—S1	115.31 (7)	C13—C18—O1	118.09 (19)
C31—P2—C24	109.20 (10)	C20—C19—O1	121.1 (2)
C31—P2—C25	101.69 (10)	C20—C19—C24	121.6 (2)
C24—P2—C25	105.89 (10)	O1—C19—C24	117.32 (19)
C31—P2—S2	114.95 (8)	C19—C20—C21	119.2 (2)
C24—P2—S2	111.32 (7)	C19—C20—H20	120.4
C25—P2—S2	113.04 (8)	C21—C20—H20	120.4
C19—O1—C18	116.50 (16)	C22—C21—C20	120.6 (2)
C2—C1—C6	119.7 (2)	C22—C21—H21	119.7
C2—C1—P1	123.61 (17)	C20—C21—H21	119.7
C6—C1—P1	116.65 (18)	C21—C22—C23	119.8 (2)
C1—C2—C3	119.8 (2)	C21—C22—H22	120.1
C1—C2—H2	120.1	C23—C22—H22	120.1
C3—C2—H2	120.1	C22—C23—C24	120.9 (2)
C4—C3—C2	120.2 (2)	C22—C23—H23	119.6
C4—C3—H3	119.9	C24—C23—H23	119.6
C2—C3—H3	119.9	C19—C24—C23	118.0 (2)
C3—C4—C5	120.1 (2)	C19—C24—P2	120.27 (16)
C3—C4—H4	120.0	C23—C24—P2	121.07 (17)
C5—C4—H4	120.0	C26—C25—C30	119.3 (2)
C6—C5—C4	120.2 (2)	C26—C25—P2	119.88 (17)
C6—C5—H5	119.9	C30—C25—P2	120.74 (17)
C4—C5—H5	119.9	C25—C26—C27	119.8 (2)

C5—C6—C1	120.0 (2)	C25—C26—H26	120.1
C5—C6—H6	120.0	C27—C26—H26	120.1
C1—C6—H6	120.0	C28—C27—C26	120.4 (2)
C12—C7—C8	119.1 (2)	C28—C27—H27	119.8
C12—C7—P1	120.97 (17)	C26—C27—H27	119.8
C8—C7—P1	119.93 (17)	C27—C28—C29	120.1 (2)
C9—C8—C7	120.5 (2)	C27—C28—H28	119.9
C9—C8—H8	119.7	C29—C28—H28	119.9
C7—C8—H8	119.7	C28—C29—C30	120.2 (2)
C10—C9—C8	119.7 (2)	C28—C29—H29	119.9
C10—C9—H9	120.1	C30—C29—H29	119.9
C8—C9—H9	120.1	C29—C30—C25	120.2 (2)
C11—C10—C9	120.1 (2)	C29—C30—H30	119.9
C11—C10—H10	120.0	C25—C30—H30	119.9
C9—C10—H10	120.0	C36—C31—C32	119.7 (2)
C10—C11—C12	120.3 (2)	C36—C31—P2	124.20 (19)
C10—C11—H11	119.9	C32—C31—P2	116.0 (2)
C12—C11—H11	119.9	C33—C32—C31	120.4 (3)
C11—C12—C7	120.2 (2)	C33—C32—H32	119.8
C11—C12—H12	119.9	C31—C32—H32	119.8
C7—C12—H12	119.9	C34—C33—C32	120.1 (3)
C18—C13—C14	116.9 (2)	C34—C33—H33	120.0
C18—C13—P1	121.25 (16)	C32—C33—H33	120.0
C14—C13—P1	121.84 (18)	C33—C34—C35	120.3 (3)
C15—C14—C13	121.5 (2)	C33—C34—H34	119.8
C15—C14—H14	119.2	C35—C34—H34	119.8
C13—C14—H14	119.2	C34—C35—C36	120.1 (3)
C16—C15—C14	119.7 (2)	C34—C35—H35	119.9
C16—C15—H15	120.1	C36—C35—H35	119.9
C14—C15—H15	120.1	C31—C36—C35	119.3 (3)
C15—C16—C17	120.4 (2)	C31—C36—H36	120.3
C15—C16—H16	119.8	C35—C36—H36	120.3
C17—C16—H16	119.8		
C7—P1—C1—C2	116.05 (19)	C18—O1—C19—C20	42.8 (3)
C13—P1—C1—C2	6.9 (2)	C18—O1—C19—C24	−139.6 (2)
S1—P1—C1—C2	−121.57 (18)	O1—C19—C20—C21	178.0 (2)
C7—P1—C1—C6	−62.03 (19)	C24—C19—C20—C21	0.4 (3)
C13—P1—C1—C6	−171.23 (17)	C19—C20—C21—C22	−1.0 (4)
S1—P1—C1—C6	60.35 (19)	C20—C21—C22—C23	0.8 (4)
C6—C1—C2—C3	0.6 (3)	C21—C22—C23—C24	0.0 (3)
P1—C1—C2—C3	−177.44 (18)	C20—C19—C24—C23	0.3 (3)
C1—C2—C3—C4	−0.4 (4)	O1—C19—C24—C23	−177.29 (19)
C2—C3—C4—C5	−0.4 (4)	C20—C19—C24—P2	−170.54 (17)
C3—C4—C5—C6	0.9 (4)	O1—C19—C24—P2	11.8 (3)
C4—C5—C6—C1	−0.7 (4)	C22—C23—C24—C19	−0.5 (3)
C2—C1—C6—C5	0.0 (3)	C22—C23—C24—P2	170.25 (17)
P1—C1—C6—C5	178.12 (19)	C31—P2—C24—C19	−70.21 (19)

C1—P1—C7—C12	139.63 (19)	C25—P2—C24—C19	−179.00 (17)
C13—P1—C7—C12	−109.22 (19)	S2—P2—C24—C19	57.77 (19)
S1—P1—C7—C12	16.5 (2)	C31—P2—C24—C23	119.20 (18)
C1—P1—C7—C8	−42.0 (2)	C25—P2—C24—C23	10.4 (2)
C13—P1—C7—C8	69.2 (2)	S2—P2—C24—C23	−112.82 (17)
S1—P1—C7—C8	−165.16 (17)	C31—P2—C25—C26	142.96 (19)
C12—C7—C8—C9	1.7 (4)	C24—P2—C25—C26	−102.96 (19)
P1—C7—C8—C9	−176.74 (19)	S2—P2—C25—C26	19.2 (2)
C7—C8—C9—C10	−0.3 (4)	C31—P2—C25—C30	−33.3 (2)
C8—C9—C10—C11	−1.3 (4)	C24—P2—C25—C30	80.8 (2)
C9—C10—C11—C12	1.5 (4)	S2—P2—C25—C30	−157.06 (16)
C10—C11—C12—C7	0.0 (3)	C30—C25—C26—C27	0.5 (3)
C8—C7—C12—C11	−1.5 (3)	P2—C25—C26—C27	−175.83 (18)
P1—C7—C12—C11	176.86 (17)	C25—C26—C27—C28	−0.4 (4)
C1—P1—C13—C18	−71.5 (2)	C26—C27—C28—C29	−0.1 (4)
C7—P1—C13—C18	−179.78 (18)	C27—C28—C29—C30	0.7 (4)
S1—P1—C13—C18	56.2 (2)	C28—C29—C30—C25	−0.7 (4)
C1—P1—C13—C14	109.3 (2)	C26—C25—C30—C29	0.1 (3)
C7—P1—C13—C14	1.0 (2)	P2—C25—C30—C29	176.34 (18)
S1—P1—C13—C14	−123.07 (18)	C24—P2—C31—C36	1.0 (2)
C18—C13—C14—C15	0.2 (3)	C25—P2—C31—C36	112.6 (2)
P1—C13—C14—C15	179.5 (2)	S2—P2—C31—C36	−124.9 (2)
C13—C14—C15—C16	1.4 (4)	C24—P2—C31—C32	−176.13 (19)
C14—C15—C16—C17	−1.0 (4)	C25—P2—C31—C32	−64.5 (2)
C15—C16—C17—C18	−1.1 (4)	S2—P2—C31—C32	57.9 (2)
C16—C17—C18—C13	2.8 (3)	C36—C31—C32—C33	−0.8 (4)
C16—C17—C18—O1	178.9 (2)	P2—C31—C32—C33	176.5 (2)
C14—C13—C18—C17	−2.4 (3)	C31—C32—C33—C34	0.7 (5)
P1—C13—C18—C17	178.35 (17)	C32—C33—C34—C35	−0.2 (5)
C14—C13—C18—O1	−178.50 (19)	C33—C34—C35—C36	−0.2 (5)
P1—C13—C18—O1	2.2 (3)	C32—C31—C36—C35	0.3 (4)
C19—O1—C18—C17	51.3 (3)	P2—C31—C36—C35	−176.8 (2)
C19—O1—C18—C13	−132.5 (2)	C34—C35—C36—C31	0.2 (4)

Hydrogen-bond geometry (Å, º)

Cg4 is the centroid of ring C19–C24.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···S2[i]	0.95	2.82	3.696 (2)	153
C4—H4···S2[ii]	0.95	2.94	3.698 (3)	138
C5—H5···S1[iii]	0.95	2.93	3.796 (3)	152
C9—H9···Cg4[iv]	0.95	2.94	3.598 (3)	127

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) *x*−1/2, −*y*+1/2, −*z*+1; (iii) *x*−1/2, *y*, −*z*+1/2; (iv) −*x*+3/2, *y*−1/2, *z*.

(2) (2-{2-[Diphenyl(selanylidene)phosphanyl]phenoxy}phenyl)diphenyl-λ^5-phosphaneselone

Crystal data

$C_{36}H_{28}OP_2Se_2$	$F(000) = 1400$
$M_r = 696.44$	$D_x = 1.510$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
$a = 14.0964$ (15) Å	Cell parameters from 13788 reflections
$b = 13.0854$ (13) Å	$\theta = 3.1$–$27.6°$
$c = 17.5918$ (18) Å	$\mu = 2.55$ mm^{-1}
$\beta = 109.226$ (8)°	$T = 173$ K
$V = 3064.0$ (6) Å^3	Prism, colorless
$Z = 4$	$0.80 \times 0.12 \times 0.12$ mm

Data collection

Rigaku XtaLAB mini diffractometer	15840 measured reflections
Radiation source: normal-focus sealed tube	3521 independent reflections
Detector resolution: 6.849 pixels mm^{-1}	2958 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.045$
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)	$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$T_{min} = 0.556$, $T_{max} = 0.737$	$h = -18 \rightarrow 18$
	$k = -16 \rightarrow 16$
	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.032$	$w = 1/[\sigma^2(F_o^2) + (0.0183P)^2 + 4.7666P]$
$wR(F^2) = 0.066$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
3521 reflections	$\Delta\rho_{max} = 0.40$ e Å^{-3}
186 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}
0 restraints	

Special details

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Se1	0.15497 (2)	0.31054 (2)	0.63637 (2)	0.02846 (8)
P1	−0.00071 (4)	0.28040 (4)	0.58870 (3)	0.01801 (12)
O1	0.0000	0.35271 (16)	0.7500	0.0191 (4)
C1	−0.03973 (16)	0.15982 (16)	0.61952 (12)	0.0201 (5)
C2	−0.10828 (17)	0.15221 (18)	0.66065 (14)	0.0267 (5)
H2	−0.1341	0.2123	0.6770	0.032*
C3	−0.13892 (19)	0.0569 (2)	0.67788 (15)	0.0336 (6)
H3	−0.1859	0.0521	0.7060	0.040*
C4	−0.10223 (19)	−0.03063 (19)	0.65480 (15)	0.0338 (6)
H4	−0.1242	−0.0956	0.6665	0.041*

C5	−0.0331 (2)	−0.02409 (19)	0.61439 (15)	0.0333 (6)
H5	−0.0075	−0.0846	0.5985	0.040*
C6	−0.00137 (18)	0.07029 (18)	0.59724 (14)	0.0284 (5)
H6	0.0468	0.0745	0.5702	0.034*
C7	−0.04357 (15)	0.27085 (16)	0.47944 (12)	0.0189 (4)
C8	−0.13290 (16)	0.22060 (18)	0.43821 (13)	0.0238 (5)
H8	−0.1715	0.1900	0.4673	0.029*
C9	−0.16556 (16)	0.21505 (18)	0.35504 (14)	0.0264 (5)
H9	−0.2261	0.1801	0.3272	0.032*
C10	−0.11013 (18)	0.26041 (18)	0.31268 (14)	0.0276 (5)
H10	−0.1332	0.2576	0.2555	0.033*
C11	−0.02133 (19)	0.30990 (19)	0.35299 (14)	0.0312 (6)
H11	0.0168	0.3407	0.3235	0.037*
C12	0.01247 (17)	0.31487 (18)	0.43633 (13)	0.0255 (5)
H12	0.0740	0.3484	0.4639	0.031*
C13	−0.07964 (15)	0.37932 (16)	0.60936 (12)	0.0191 (4)
C14	−0.15170 (16)	0.43227 (17)	0.54724 (14)	0.0237 (5)
H14	−0.1613	0.4148	0.4928	0.028*
C15	−0.20897 (16)	0.50950 (17)	0.56408 (15)	0.0269 (5)
H15	−0.2571	0.5447	0.5213	0.032*
C16	−0.19615 (16)	0.53555 (17)	0.64311 (15)	0.0267 (5)
H16	−0.2361	0.5880	0.6545	0.032*
C17	−0.12510 (16)	0.48518 (17)	0.70579 (14)	0.0227 (5)
H17	−0.1160	0.5031	0.7601	0.027*
C18	−0.06746 (15)	0.40848 (16)	0.68848 (13)	0.0188 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.01582 (11)	0.04058 (16)	0.02624 (13)	−0.00167 (10)	0.00320 (9)	−0.00400 (11)
P1	0.0159 (3)	0.0209 (3)	0.0167 (3)	−0.0006 (2)	0.0045 (2)	0.0003 (2)
O1	0.0205 (10)	0.0157 (10)	0.0196 (10)	0.000	0.0047 (9)	0.000
C1	0.0214 (11)	0.0192 (11)	0.0178 (10)	0.0017 (8)	0.0037 (9)	0.0022 (8)
C2	0.0281 (12)	0.0227 (12)	0.0325 (13)	−0.0018 (9)	0.0142 (11)	−0.0006 (10)
C3	0.0355 (14)	0.0317 (15)	0.0396 (15)	−0.0068 (11)	0.0202 (12)	0.0012 (11)
C4	0.0409 (14)	0.0209 (13)	0.0363 (14)	−0.0047 (11)	0.0084 (12)	0.0064 (10)
C5	0.0453 (15)	0.0202 (13)	0.0329 (13)	0.0092 (11)	0.0108 (12)	0.0022 (10)
C6	0.0312 (13)	0.0279 (13)	0.0281 (12)	0.0063 (10)	0.0126 (10)	0.0038 (10)
C7	0.0194 (10)	0.0193 (11)	0.0172 (10)	−0.0004 (8)	0.0047 (8)	0.0005 (8)
C8	0.0191 (11)	0.0285 (13)	0.0233 (11)	−0.0044 (9)	0.0064 (9)	−0.0018 (9)
C9	0.0192 (11)	0.0282 (13)	0.0272 (12)	−0.0004 (9)	0.0013 (9)	−0.0034 (10)
C10	0.0347 (13)	0.0273 (13)	0.0178 (11)	0.0008 (10)	0.0047 (10)	0.0019 (9)
C11	0.0386 (14)	0.0326 (14)	0.0244 (12)	−0.0083 (11)	0.0129 (11)	0.0066 (10)
C12	0.0253 (11)	0.0257 (12)	0.0246 (11)	−0.0089 (10)	0.0071 (9)	0.0002 (10)
C13	0.0170 (10)	0.0166 (11)	0.0225 (11)	−0.0018 (8)	0.0049 (9)	0.0009 (9)
C14	0.0208 (11)	0.0234 (12)	0.0240 (11)	−0.0027 (9)	0.0035 (9)	0.0032 (9)
C15	0.0191 (11)	0.0208 (12)	0.0353 (13)	0.0007 (9)	0.0018 (10)	0.0059 (10)
C16	0.0199 (11)	0.0184 (12)	0.0411 (14)	0.0014 (9)	0.0091 (10)	−0.0010 (10)

C17	0.0215 (11)	0.0192 (11)	0.0282 (12)	−0.0038 (9)	0.0090 (10)	−0.0029 (9)
C18	0.0167 (10)	0.0161 (11)	0.0232 (11)	−0.0028 (8)	0.0058 (9)	0.0027 (8)

Geometric parameters (Å, º)

Se1—P1	2.1125 (6)	C8—C9	1.384 (3)
P1—C1	1.812 (2)	C8—H8	0.9500
P1—C7	1.819 (2)	C9—C10	1.379 (3)
P1—C13	1.820 (2)	C9—H9	0.9500
O1—C18	1.389 (2)	C10—C11	1.380 (3)
O1—C18[i]	1.389 (2)	C10—H10	0.9500
C1—C2	1.388 (3)	C11—C12	1.386 (3)
C1—C6	1.399 (3)	C11—H11	0.9500
C2—C3	1.385 (3)	C12—H12	0.9500
C2—H2	0.9500	C13—C18	1.398 (3)
C3—C4	1.372 (4)	C13—C14	1.405 (3)
C3—H3	0.9500	C14—C15	1.385 (3)
C4—C5	1.385 (4)	C14—H14	0.9500
C4—H4	0.9500	C15—C16	1.384 (3)
C5—C6	1.380 (3)	C15—H15	0.9500
C5—H5	0.9500	C16—C17	1.388 (3)
C6—H6	0.9500	C16—H16	0.9500
C7—C12	1.387 (3)	C17—C18	1.387 (3)
C7—C8	1.394 (3)	C17—H17	0.9500
C1—P1—C7	103.20 (10)	C10—C9—C8	119.9 (2)
C1—P1—C13	107.09 (10)	C10—C9—H9	120.1
C7—P1—C13	104.34 (10)	C8—C9—H9	120.1
C1—P1—Se1	114.95 (7)	C9—C10—C11	120.2 (2)
C7—P1—Se1	111.86 (7)	C9—C10—H10	119.9
C13—P1—Se1	114.30 (7)	C11—C10—H10	119.9
C18—O1—C18[i]	116.6 (2)	C10—C11—C12	120.2 (2)
C2—C1—C6	119.0 (2)	C10—C11—H11	119.9
C2—C1—P1	123.39 (17)	C12—C11—H11	119.9
C6—C1—P1	117.51 (17)	C11—C12—C7	120.0 (2)
C3—C2—C1	119.9 (2)	C11—C12—H12	120.0
C3—C2—H2	120.0	C7—C12—H12	120.0
C1—C2—H2	120.0	C18—C13—C14	117.4 (2)
C4—C3—C2	120.8 (2)	C18—C13—P1	120.67 (16)
C4—C3—H3	119.6	C14—C13—P1	121.89 (17)
C2—C3—H3	119.6	C15—C14—C13	121.1 (2)
C3—C4—C5	119.8 (2)	C15—C14—H14	119.5
C3—C4—H4	120.1	C13—C14—H14	119.5
C5—C4—H4	120.1	C16—C15—C14	120.1 (2)
C6—C5—C4	120.1 (2)	C16—C15—H15	119.9
C6—C5—H5	120.0	C14—C15—H15	119.9
C4—C5—H5	120.0	C15—C16—C17	120.2 (2)
C5—C6—C1	120.3 (2)	C15—C16—H16	119.9

C5—C6—H6	119.8	C17—C16—H16	119.9
C1—C6—H6	119.8	C18—C17—C16	119.4 (2)
C12—C7—C8	119.4 (2)	C18—C17—H17	120.3
C12—C7—P1	119.88 (16)	C16—C17—H17	120.3
C8—C7—P1	120.72 (16)	C17—C18—O1	120.62 (19)
C9—C8—C7	120.3 (2)	C17—C18—C13	121.83 (19)
C9—C8—H8	119.9	O1—C18—C13	117.40 (18)
C7—C8—H8	119.9		
C7—P1—C1—C2	−117.40 (19)	C9—C10—C11—C12	−0.4 (4)
C13—P1—C1—C2	−7.6 (2)	C10—C11—C12—C7	−0.6 (4)
Se1—P1—C1—C2	120.53 (18)	C8—C7—C12—C11	1.0 (4)
C7—P1—C1—C6	59.79 (19)	P1—C7—C12—C11	−178.38 (19)
C13—P1—C1—C6	169.57 (17)	C1—P1—C13—C18	71.55 (19)
Se1—P1—C1—C6	−62.27 (18)	C7—P1—C13—C18	−179.48 (17)
C6—C1—C2—C3	−1.0 (3)	Se1—P1—C13—C18	−57.00 (18)
P1—C1—C2—C3	176.11 (18)	C1—P1—C13—C14	−111.23 (18)
C1—C2—C3—C4	0.1 (4)	C7—P1—C13—C14	−2.2 (2)
C2—C3—C4—C5	0.5 (4)	Se1—P1—C13—C14	120.23 (16)
C3—C4—C5—C6	−0.1 (4)	C18—C13—C14—C15	−0.7 (3)
C4—C5—C6—C1	−0.9 (4)	P1—C13—C14—C15	−177.99 (17)
C2—C1—C6—C5	1.5 (3)	C13—C14—C15—C16	−0.3 (3)
P1—C1—C6—C5	−175.86 (18)	C14—C15—C16—C17	0.7 (3)
C1—P1—C7—C12	−145.39 (19)	C15—C16—C17—C18	−0.2 (3)
C13—P1—C7—C12	102.79 (19)	C16—C17—C18—O1	−176.18 (19)
Se1—P1—C7—C12	−21.3 (2)	C16—C17—C18—C13	−0.8 (3)
C1—P1—C7—C8	35.3 (2)	C18^i—O1—C18—C17	−51.46 (16)
C13—P1—C7—C8	−76.5 (2)	C18^i—O1—C18—C13	132.9 (2)
Se1—P1—C7—C8	159.41 (16)	C14—C13—C18—C17	1.2 (3)
C12—C7—C8—C9	−0.3 (3)	P1—C13—C18—C17	178.56 (16)
P1—C7—C8—C9	179.05 (17)	C14—C13—C18—O1	176.74 (17)
C7—C8—C9—C10	−0.7 (3)	P1—C13—C18—O1	−5.9 (3)
C8—C9—C10—C11	1.1 (4)		

Symmetry code: (i) −x, y, −z+3/2.

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are the centroids of rings C7–C12 and C13–C18, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···*Cg*2^{ii}	0.95	2.63	3.546 (3)	161
C9—H9···*Cg*3^{iii}	0.95	2.94	3.676 (3)	135

Symmetry codes: (ii) −x, −y+1, −z+1; (iii) −x−1/2, −y+1/2, −z+1.