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1,2-Bis(Diphenylphosphinoselenoyl)-ethane

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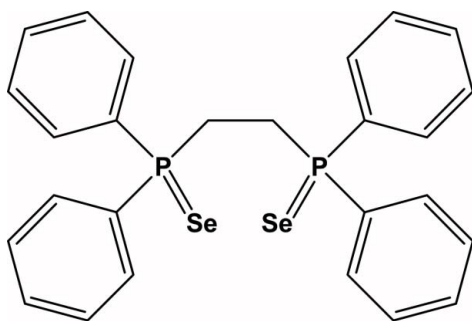
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Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.052; wR factor = 0.160; data-to-parameter ratio = 15.1.

In the title compound, $(\text{CH}_2)_2(\text{PPh}_2)_2\text{Se}_2$ or $\text{C}_{26}\text{H}_{24}\text{P}_2\text{Se}_2$, there are two half-molecules in the asymmetric unit, both molecules having inversion symmetry. The P–Se bond lengths suggest weak double-bond character. Weak C–H...Se hydrogen bonds help to assemble the molecules into a three-dimensional network.

Related literature

For further details, see: Risto *et al.* (2007). For a related structure and background, see: Brown *et al.* (1980). For reference structural data, see: Emsley (1998).



Experimental

Crystal data

$\text{C}_{26}\text{H}_{24}\text{P}_2\text{Se}_2$
 $M_r = 556.31$
 Triclinic, $P\bar{1}$
 $a = 10.322$ (2) Å
 $b = 10.843$ (2) Å
 $c = 12.285$ (3) Å
 $\alpha = 90.93$ (3)°
 $\beta = 108.13$ (3)°

$\gamma = 112.14$ (3)°
 $V = 1196.3$ (4) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 3.24$ mm⁻¹
 $T = 120$ (2) K
 $0.10 \times 0.10 \times 0.05$ mm

Data collection

Nonius KappaCCD area-detector diffractometer
 Absorption correction: multi-scan (*XPREP* in *SHELXTL*; Bruker, 2001)
 $T_{\min} = 0.738$, $T_{\max} = 0.855$
 14810 measured reflections
 4095 independent reflections
 3328 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.099$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.160$
 $S = 1.11$
 4095 reflections
 271 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.58$ e Å⁻³
 $\Delta\rho_{\min} = -0.75$ e Å⁻³

Table 1

Selected bond lengths (Å).

P1–Se1	2.1093 (19)	P2–Se2	2.1042 (16)
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Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C15–H15...Se1 ⁱ	0.95	3.03	3.732 (6)	132
C25–H25...Se2 ⁱⁱ	0.95	3.01	3.954 (6)	171
C14–H14...Se2 ⁱⁱⁱ	0.95	2.98	3.690 (7)	133
C24–H24...Se2 ^{iv}	0.95	2.99	3.751 (6)	138

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2546).

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supplementary materials

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1,2-Bis(Diphenylphosphinoselenoyl)ethane

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Comment

The crystals of the title compound, (I), $(\text{CH}_2)_2(\text{PPh}_2)_2\text{Se}_2$, were isolated as a side product during the synthesis (Risto *et al.*, 2007) of $[\text{Pd}(\text{SeC}_4\text{H}_4\text{S})_2(\text{dppe})]$ (dppe = diphenylphosphine) from $[\text{PdCl}_2(\text{dppe})]$ and $\text{LiSeC}_4\text{H}_4\text{S}$ (prepared from thiophene, *n*-butyllithium, and an excess of elemental selenium). The asymmetric unit of (I) consists of two independent half-molecules, both molecular environments being completed by crystallographic inversion symmetry (Fig. 1). The two independent P—Se bond lengths are 2.104 (2) and 2.109 (2) Å indicating a slight double bond character [the sum of the covalent radii of phosphorus and selenium is 2.22 Å (Emsley 1998)]. The other bonds show normal single bond lengths. The molecules are assembled into a three-dimensional network by weak C—H \cdots Se interactions (Table 2, Fig. 2).

Experimental

The crystals of the title compound were isolated in synthesis of $[\text{Pd}(\text{SeC}_4\text{H}_4\text{S})_2(\text{dppe})]$ from $[\text{PdCl}_2(\text{dppe})]$ (0.387 g, 0.673 mmol, in 15 ml dichloromethane) and lithium 2-thienylselenolate (1.474 mmol in 4.1 ml tetrahydrofuran, prepared from thiophene, *n*-butyllithium, and an excess of elemental selenium; used *in situ*). Colourless plates of (I) were obtained from the reaction mixture.

Refinement

The H atoms were positioned geometrically (C—H = 0.95–0.98 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

Figures

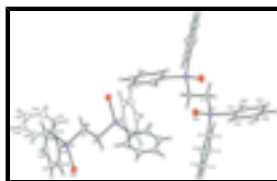


Fig. 1. The molecular structure of (I) with displacement ellipsoids for the non-hydrogen atoms drawn at the 50% probability limit. The unlabelled atoms in the C1 and C2 molecule are generated by the symmetry operations $(-x, -y, 2 - z)$ and $(-x, 1 - y, 1 - z)$, respectively.

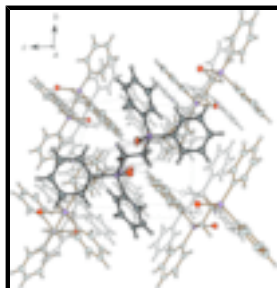


Fig. 2. The packing of molecules in (I) with C—H \cdots Se interactions indicated by dashed lines.

1,2-bis(Diphenylphosphinoselenoyl)ethane

Crystal data

$C_{26}H_{24}P_2Se_2$	$Z = 2$
$M_r = 556.31$	$F_{000} = 556$
Triclinic, $P\bar{1}$	$D_x = 1.544 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 10.322 (2) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 10.843 (2) \text{ \AA}$	Cell parameters from 3328 reflections
$c = 12.285 (3) \text{ \AA}$	$\theta = 2.3\text{--}25.0^\circ$
$\alpha = 90.93 (3)^\circ$	$\mu = 3.24 \text{ mm}^{-1}$
$\beta = 108.13 (3)^\circ$	$T = 120 (2) \text{ K}$
$\gamma = 112.14 (3)^\circ$	Plate, colourless
$V = 1196.3 (4) \text{ \AA}^3$	$0.10 \times 0.10 \times 0.05 \text{ mm}$

Data collection

Nonius KappaCCD area-detector diffractometer	4095 independent reflections
Radiation source: fine-focus sealed tube	3328 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.099$
$T = 120(2) \text{ K}$	$\theta_{\text{max}} = 25.0^\circ$
φ scans, and ω scans with κ offsets	$\theta_{\text{min}} = 2.3^\circ$
Absorption correction: multi-scan (XPREP in SHELXTL; Bruker, 2001)	$h = -12 \rightarrow 12$
$T_{\text{min}} = 0.738$, $T_{\text{max}} = 0.855$	$k = -12 \rightarrow 12$
14810 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained
$wR(F^2) = 0.160$	$w = 1/[\sigma^2(F_o^2) + (0.0852P)^2 + 2.3976P]$
$S = 1.11$	where $P = (F_o^2 + 2F_c^2)/3$
4095 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
271 parameters	$\Delta\rho_{\text{max}} = 0.58 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.75 \text{ e \AA}^{-3}$
	Extinction correction: none

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.

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>	$U_{\text{iso}}^*/U_{\text{eq}}$
Se1	0.37097 (7)	0.12472 (6)	1.09921 (5)	0.0283 (2)
Se2	0.76343 (7)	0.38570 (6)	0.51739 (5)	0.0245 (2)
P1	0.19425 (17)	0.09757 (15)	0.94441 (13)	0.0179 (3)
P2	0.60174 (16)	0.36746 (14)	0.59353 (13)	0.0172 (3)
C1	0.0226 (7)	0.0653 (6)	0.9721 (5)	0.0212 (13)
H1A	0.0360	0.1426	1.0248	0.025*
H1B	-0.0577	0.0553	0.8985	0.025*
C2	0.5289 (7)	0.4973 (6)	0.5655 (5)	0.0202 (12)
H2A	0.4468	0.4785	0.5967	0.024*
H2B	0.6085	0.5859	0.6060	0.024*
C11	0.1511 (6)	-0.0439 (6)	0.8372 (5)	0.0168 (12)
C12	0.0077 (7)	-0.1131 (6)	0.7594 (5)	0.0243 (13)
H12	-0.0697	-0.0870	0.7616	0.029*
C13	-0.0230 (7)	-0.2195 (6)	0.6788 (5)	0.0251 (14)
H13	-0.1215	-0.2672	0.6263	0.030*
C14	0.0889 (7)	-0.2562 (6)	0.6748 (5)	0.0264 (14)
H14	0.0674	-0.3303	0.6201	0.032*
C15	0.2308 (7)	-0.1869 (6)	0.7489 (5)	0.0264 (14)
H15	0.3079	-0.2120	0.7442	0.032*
C16	0.2642 (7)	-0.0800 (6)	0.8311 (6)	0.0259 (14)
H16	0.3633	-0.0323	0.8825	0.031*
C21	0.2249 (6)	0.2447 (5)	0.8708 (5)	0.0173 (12)
C22	0.3695 (7)	0.3401 (6)	0.8960 (5)	0.0219 (13)
H22	0.4509	0.3281	0.9502	0.026*
C23	0.3934 (7)	0.4541 (6)	0.8404 (5)	0.0255 (14)
H23	0.4918	0.5199	0.8569	0.031*
C24	0.2746 (8)	0.4717 (6)	0.7614 (5)	0.0277 (15)
H24	0.2920	0.5492	0.7239	0.033*
C25	0.1316 (8)	0.3772 (6)	0.7374 (6)	0.0301 (15)
H25	0.0501	0.3897	0.6840	0.036*
C26	0.1073 (7)	0.2630 (6)	0.7919 (5)	0.0264 (14)
H26	0.0089	0.1970	0.7747	0.032*
C31	0.4360 (7)	0.2109 (6)	0.5413 (5)	0.0190 (12)

supplementary materials

C32	0.3272 (7)	0.1831 (6)	0.5921 (5)	0.0235 (13)
H32	0.3376	0.2484	0.6503	0.028*
C33	0.2047 (7)	0.0625 (6)	0.5595 (5)	0.0274 (14)
H33	0.1324	0.0433	0.5964	0.033*
C34	0.1881 (7)	-0.0310 (6)	0.4719 (6)	0.0286 (15)
H34	0.1037	-0.1145	0.4485	0.034*
C35	0.2937 (7)	-0.0027 (6)	0.4188 (6)	0.0303 (15)
H35	0.2811	-0.0668	0.3586	0.036*
C36	0.4176 (7)	0.1178 (6)	0.4524 (5)	0.0237 (13)
H36	0.4896	0.1370	0.4152	0.028*
C41	0.6711 (6)	0.3761 (6)	0.7497 (5)	0.0182 (12)
C42	0.7566 (7)	0.5016 (6)	0.8218 (5)	0.0255 (14)
H42	0.7743	0.5828	0.7894	0.031*
C43	0.8148 (8)	0.5053 (7)	0.9404 (6)	0.0314 (15)
H43	0.8712	0.5896	0.9896	0.038*
C44	0.7916 (8)	0.3880 (7)	0.9876 (6)	0.0299 (15)
H44	0.8316	0.3916	1.0691	0.036*
C45	0.7107 (8)	0.2655 (7)	0.9171 (5)	0.0308 (15)
H45	0.6963	0.1849	0.9501	0.037*
C46	0.6504 (7)	0.2584 (6)	0.7992 (5)	0.0256 (14)
H46	0.5946	0.1732	0.7513	0.031*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.0319 (4)	0.0263 (4)	0.0202 (4)	0.0109 (3)	0.0013 (3)	0.0036 (3)
Se2	0.0223 (4)	0.0299 (4)	0.0237 (4)	0.0112 (3)	0.0101 (3)	0.0055 (3)
P1	0.0202 (8)	0.0160 (7)	0.0177 (8)	0.0061 (6)	0.0080 (6)	0.0042 (6)
P2	0.0197 (8)	0.0165 (8)	0.0156 (8)	0.0078 (6)	0.0057 (6)	0.0043 (6)
C1	0.029 (3)	0.019 (3)	0.028 (3)	0.014 (3)	0.021 (3)	0.012 (3)
C2	0.021 (3)	0.015 (3)	0.018 (3)	0.005 (2)	0.002 (2)	0.002 (2)
C11	0.017 (3)	0.021 (3)	0.015 (3)	0.007 (2)	0.008 (2)	0.007 (2)
C12	0.022 (3)	0.028 (3)	0.027 (3)	0.010 (3)	0.013 (3)	0.012 (3)
C13	0.024 (3)	0.022 (3)	0.020 (3)	0.001 (3)	0.005 (3)	-0.001 (3)
C14	0.034 (4)	0.021 (3)	0.021 (3)	0.006 (3)	0.013 (3)	-0.001 (3)
C15	0.030 (4)	0.028 (3)	0.027 (3)	0.015 (3)	0.014 (3)	0.003 (3)
C16	0.021 (3)	0.025 (3)	0.032 (4)	0.009 (3)	0.009 (3)	0.005 (3)
C21	0.021 (3)	0.013 (3)	0.018 (3)	0.004 (2)	0.010 (2)	-0.002 (2)
C22	0.025 (3)	0.022 (3)	0.021 (3)	0.010 (3)	0.010 (3)	0.001 (2)
C23	0.033 (4)	0.018 (3)	0.030 (4)	0.007 (3)	0.019 (3)	0.003 (3)
C24	0.046 (4)	0.016 (3)	0.024 (3)	0.012 (3)	0.016 (3)	0.006 (3)
C25	0.034 (4)	0.028 (4)	0.026 (4)	0.013 (3)	0.007 (3)	0.011 (3)
C26	0.022 (3)	0.019 (3)	0.028 (4)	0.000 (3)	0.007 (3)	0.002 (3)
C31	0.025 (3)	0.014 (3)	0.018 (3)	0.009 (3)	0.006 (2)	0.004 (2)
C32	0.023 (3)	0.022 (3)	0.022 (3)	0.007 (3)	0.007 (3)	0.001 (3)
C33	0.026 (3)	0.025 (3)	0.025 (3)	0.004 (3)	0.009 (3)	0.003 (3)
C34	0.025 (3)	0.024 (3)	0.026 (4)	0.005 (3)	0.001 (3)	0.009 (3)
C35	0.031 (4)	0.019 (3)	0.033 (4)	0.007 (3)	0.004 (3)	-0.010 (3)

C36	0.021 (3)	0.024 (3)	0.025 (3)	0.011 (3)	0.004 (3)	0.004 (3)
C41	0.018 (3)	0.019 (3)	0.020 (3)	0.008 (2)	0.009 (2)	0.007 (2)
C42	0.031 (4)	0.019 (3)	0.025 (3)	0.011 (3)	0.008 (3)	0.005 (3)
C43	0.037 (4)	0.030 (4)	0.025 (4)	0.014 (3)	0.007 (3)	0.006 (3)
C44	0.036 (4)	0.038 (4)	0.017 (3)	0.017 (3)	0.007 (3)	0.009 (3)
C45	0.038 (4)	0.035 (4)	0.022 (4)	0.020 (3)	0.008 (3)	0.012 (3)
C46	0.032 (4)	0.021 (3)	0.020 (3)	0.011 (3)	0.004 (3)	0.005 (3)

Geometric parameters (Å, °)

P1—Se1	2.1093 (19)	C23—C24	1.387 (9)
P2—Se2	2.1042 (16)	C23—H23	0.9500
P1—C1	1.814 (6)	C24—C25	1.377 (9)
P1—C21	1.819 (6)	C24—H24	0.9500
P1—C11	1.828 (6)	C25—C26	1.394 (9)
P2—C41	1.814 (6)	C25—H25	0.9500
P2—C31	1.820 (6)	C26—H26	0.9500
P2—C2	1.822 (6)	C31—C32	1.389 (8)
C1—C1 ⁱ	1.557 (11)	C31—C36	1.392 (8)
C1—H1A	0.9900	C32—C33	1.375 (9)
C1—H1B	0.9900	C32—H32	0.9500
C2—C2 ⁱⁱ	1.544 (11)	C33—C34	1.390 (9)
C2—H2A	0.9900	C33—H33	0.9500
C2—H2B	0.9900	C34—C35	1.380 (10)
C11—C16	1.385 (8)	C34—H34	0.9500
C11—C12	1.388 (8)	C35—C36	1.382 (9)
C12—C13	1.379 (9)	C35—H35	0.9500
C12—H12	0.9500	C36—H36	0.9500
C13—C14	1.369 (9)	C41—C46	1.394 (8)
C13—H13	0.9500	C41—C42	1.409 (8)
C14—C15	1.363 (9)	C42—C43	1.387 (9)
C14—H14	0.9500	C42—H42	0.9500
C15—C16	1.387 (9)	C43—C44	1.376 (9)
C15—H15	0.9500	C43—H43	0.9500
C16—H16	0.9500	C44—C45	1.374 (10)
C21—C26	1.380 (9)	C44—H44	0.9500
C21—C22	1.390 (8)	C45—C46	1.375 (9)
C22—C23	1.399 (9)	C45—H45	0.9500
C22—H22	0.9500	C46—H46	0.9500
C1—P1—C21	105.2 (3)	C24—C23—C22	120.5 (6)
C1—P1—C11	105.5 (3)	C24—C23—H23	119.7
C21—P1—C11	106.3 (2)	C22—C23—H23	119.7
C1—P1—Se1	111.2 (2)	C25—C24—C23	120.2 (6)
C21—P1—Se1	113.4 (2)	C25—C24—H24	119.9
C11—P1—Se1	114.52 (19)	C23—C24—H24	119.9
C41—P2—C31	105.4 (3)	C24—C25—C26	119.5 (6)
C41—P2—C2	106.5 (3)	C24—C25—H25	120.3
C31—P2—C2	103.7 (3)	C26—C25—H25	120.3

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C41—P2—Se2	112.92 (19)	C21—C26—C25	120.7 (6)
C31—P2—Se2	114.43 (19)	C21—C26—H26	119.7
C2—P2—Se2	113.1 (2)	C25—C26—H26	119.7
C1 ⁱ —C1—P1	110.4 (5)	C32—C31—C36	119.6 (6)
C1 ⁱ —C1—H1A	109.6	C32—C31—P2	119.4 (4)
P1—C1—H1A	109.6	C36—C31—P2	121.0 (5)
C1 ⁱ —C1—H1B	109.6	C33—C32—C31	121.0 (6)
P1—C1—H1B	109.6	C33—C32—H32	119.5
H1A—C1—H1B	108.1	C31—C32—H32	119.5
C2 ⁱⁱ —C2—P2	111.1 (5)	C32—C33—C34	119.2 (6)
C2 ⁱⁱ —C2—H2A	109.4	C32—C33—H33	120.4
P2—C2—H2A	109.4	C34—C33—H33	120.4
C2 ⁱⁱ —C2—H2B	109.4	C35—C34—C33	120.2 (6)
P2—C2—H2B	109.4	C35—C34—H34	119.9
H2A—C2—H2B	108.0	C33—C34—H34	119.9
C16—C11—C12	119.4 (5)	C34—C35—C36	120.7 (6)
C16—C11—P1	119.5 (4)	C34—C35—H35	119.7
C12—C11—P1	121.1 (4)	C36—C35—H35	119.7
C13—C12—C11	120.4 (6)	C35—C36—C31	119.4 (6)
C13—C12—H12	119.8	C35—C36—H36	120.3
C11—C12—H12	119.8	C31—C36—H36	120.3
C14—C13—C12	119.8 (6)	C46—C41—C42	119.1 (5)
C14—C13—H13	120.1	C46—C41—P2	120.3 (4)
C12—C13—H13	120.1	C42—C41—P2	120.4 (4)
C15—C14—C13	120.3 (6)	C43—C42—C41	119.3 (6)
C15—C14—H14	119.8	C43—C42—H42	120.4
C13—C14—H14	119.8	C41—C42—H42	120.4
C14—C15—C16	120.9 (6)	C44—C43—C42	120.6 (6)
C14—C15—H15	119.6	C44—C43—H43	119.7
C16—C15—H15	119.6	C42—C43—H43	119.7
C11—C16—C15	119.2 (6)	C45—C44—C43	120.1 (6)
C11—C16—H16	120.4	C45—C44—H44	120.0
C15—C16—H16	120.4	C43—C44—H44	120.0
C26—C21—C22	120.1 (5)	C44—C45—C46	120.7 (6)
C26—C21—P1	121.1 (4)	C44—C45—H45	119.7
C22—C21—P1	118.8 (5)	C46—C45—H45	119.7
C21—C22—C23	119.0 (6)	C45—C46—C41	120.2 (6)
C21—C22—H22	120.5	C45—C46—H46	119.9
C23—C22—H22	120.5	C41—C46—H46	119.9
C21—P1—C1—C1 ⁱ	176.1 (6)	C22—C21—C26—C25	-0.5 (9)
C11—P1—C1—C1 ⁱ	64.0 (6)	P1—C21—C26—C25	178.9 (5)
Se1—P1—C1—C1 ⁱ	-60.7 (6)	C24—C25—C26—C21	0.9 (10)
C41—P2—C2—C2 ⁱⁱ	178.1 (5)	C41—P2—C31—C32	50.1 (5)
C31—P2—C2—C2 ⁱⁱ	-70.9 (6)	C2—P2—C31—C32	-61.6 (5)
Se2—P2—C2—C2 ⁱⁱ	53.6 (6)	Se2—P2—C31—C32	174.8 (4)
C1—P1—C11—C16	-154.2 (5)	C41—P2—C31—C36	-128.9 (5)

C21—P1—C11—C16	94.5 (5)	C2—P2—C31—C36	119.4 (5)
Se1—P1—C11—C16	-31.5 (5)	Se2—P2—C31—C36	-4.2 (5)
C1—P1—C11—C12	27.9 (5)	C36—C31—C32—C33	2.8 (9)
C21—P1—C11—C12	-83.5 (5)	P2—C31—C32—C33	-176.2 (5)
Se1—P1—C11—C12	150.5 (4)	C31—C32—C33—C34	-1.9 (10)
C16—C11—C12—C13	1.9 (9)	C32—C33—C34—C35	0.2 (10)
P1—C11—C12—C13	179.9 (5)	C33—C34—C35—C36	0.5 (10)
C11—C12—C13—C14	-0.7 (9)	C34—C35—C36—C31	0.5 (10)
C12—C13—C14—C15	-0.9 (9)	C32—C31—C36—C35	-2.1 (9)
C13—C14—C15—C16	1.3 (10)	P2—C31—C36—C35	176.9 (5)
C12—C11—C16—C15	-1.5 (9)	C31—P2—C41—C46	31.2 (5)
P1—C11—C16—C15	-179.5 (5)	C2—P2—C41—C46	140.9 (5)
C14—C15—C16—C11	-0.1 (9)	Se2—P2—C41—C46	-94.4 (5)
C1—P1—C21—C26	-37.1 (5)	C31—P2—C41—C42	-153.9 (5)
C11—P1—C21—C26	74.4 (5)	C2—P2—C41—C42	-44.2 (5)
Se1—P1—C21—C26	-158.9 (4)	Se2—P2—C41—C42	80.4 (5)
C1—P1—C21—C22	142.3 (5)	C46—C41—C42—C43	-1.8 (9)
C11—P1—C21—C22	-106.2 (5)	P2—C41—C42—C43	-176.7 (5)
Se1—P1—C21—C22	20.5 (5)	C41—C42—C43—C44	1.0 (10)
C26—C21—C22—C23	0.0 (8)	C42—C43—C44—C45	0.3 (10)
P1—C21—C22—C23	-179.4 (4)	C43—C44—C45—C46	-0.9 (10)
C21—C22—C23—C24	0.1 (9)	C44—C45—C46—C41	0.1 (10)
C22—C23—C24—C25	0.3 (9)	C42—C41—C46—C45	1.2 (9)
C23—C24—C25—C26	-0.7 (9)	P2—C41—C46—C45	176.2 (5)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C15—H15 \cdots Se1 ⁱⁱⁱ	0.95	3.03	3.732 (6)	132
C25—H25 \cdots Se2 ^{iv}	0.95	3.01	3.954 (6)	171
C14—H14 \cdots Se2 ^v	0.95	2.98	3.690 (7)	133
C24—H24 \cdots Se2 ⁱⁱ	0.95	2.99	3.751 (6)	138

Symmetry codes: (iii) $-x+1, -y, -z+2$; (iv) $x-1, y, z$; (v) $-x+1, -y, -z+1$; (ii) $-x+1, -y+1, -z+1$.

Fig. 1

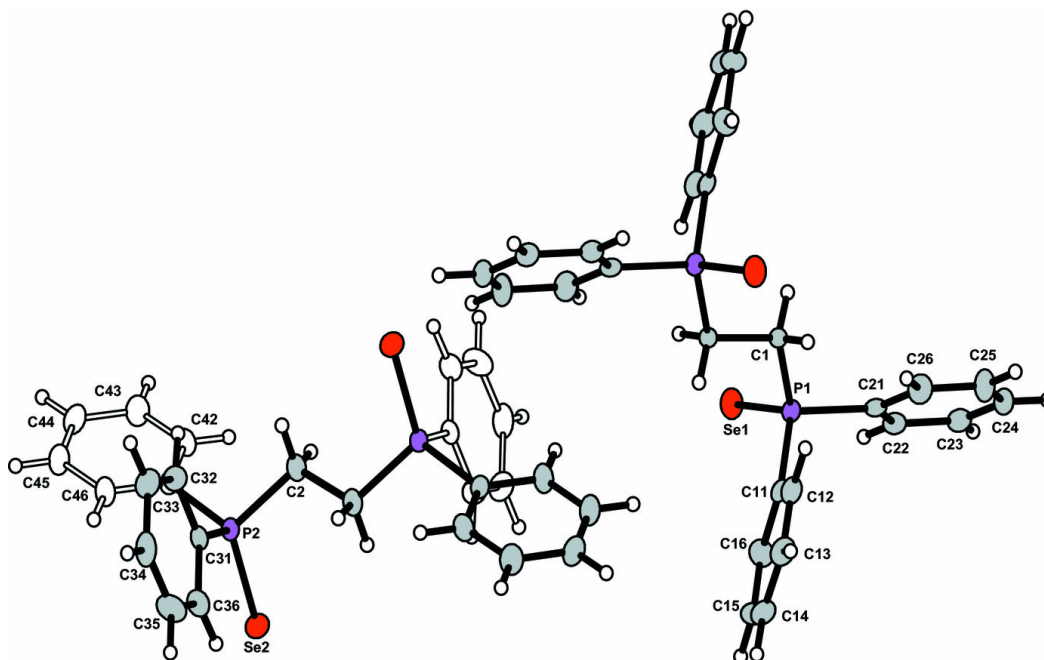


Fig. 2

