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Diphenylphosphane selenide

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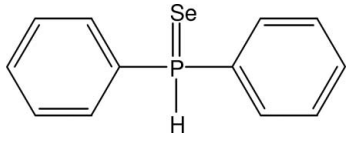
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.107; data-to-parameter ratio = 16.6.

The title compound, $C_{12}H_{11}PSe$, crystallizes with two molecules in the asymmetric unit. The bond lengths and angles of these two molecules are similar but they differ significantly in the dihedral angle between the two phenyl rings [72.70 (10) and 82.07 (9)°]. The molecules are connected by P—H···Se hydrogen bonds into zigzag chains running along the *a* axis.

Related literature

For related literature, see: Dornhaus *et al.* (2006).



Experimental

Crystal data

$C_{12}H_{11}PSe$
M_r = 265.14
Monoclinic, $P2_1/c$
a = 6.0901 (3) Å
b = 32.3775 (18) Å
c = 11.5057 (6) Å
β = 96.741 (4)°
V = 2253.0 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.43 mm^{-1}
T = 173 (2) K
0.39 × 0.22 × 0.18 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.348, T_{max} = 0.577 (expected range = 0.325–0.539)
31769 measured reflections
4221 independent reflections
3625 reflections with $I > 2\sigma(I)$
R_{int} = 0.071

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.107
S = 1.04
4221 reflections
255 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
P1A—H1A···Se1^{i}	1.32	2.87	3.7458 (9)	123
P1—H1···Se1A^{ii}	1.35	2.93	3.9652 (9)	132

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2507).

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supplementary materials

Acta Cryst. (2007). E**63**, o4917 [**doi:10.1107/S1600536807062575**]

Diphenylphosphane selenide

F. Dornhaus, H.-W. Lerner and M. Bolte

Comment

Transition metal complexes with phosphine ligands, PR_3 (R = alkyl, aryl, H) play a big role in homogeneous catalysis. A disadvantage of these ligands is their air sensitivity. Phosphoranes and phosphine chalcogenides are to be found compared with phosphines much more stable toward air oxidation. We report here the synthesis and the X-ray crystal structure analysis of Ph_2HPSe (Ph = C_6H_5). The synthesis of the title compound was achieved by the reaction of Ph_2PH (Dornhaus *et al.*, 2006) with grey Se in THF at room temperature as indicated in the equation below.

The title compound, $C_{12}H_{11}PSe$, crystallizes with two molecules in the asymmetric unit. Bond lengths and angles of these two molecules are similar but they differ significantly in the dihedral angle between the two phenyl rings [72.70 (10)° and 82.07 (9)°, respectively]. The molecules are connected by P—H···Se hydrogen bonds to zigzag chains running along the *a* axis.

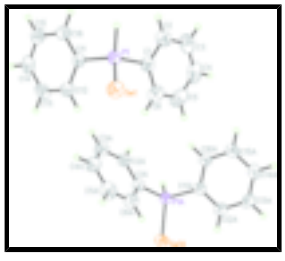
Experimental

A mixture of diphenylphosphine Ph_2PH (1.5 g, 8 mmol) and grey Se (1.0 g, 12.7 mmol) in 10 ml tetrahydrofuran was stirred for 24 h at room temperature. After filtering single crystals of Ph_2HPSe were obtained from the filtrate at room temperature (yield 70%).

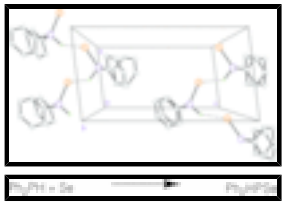
Refinement

H atoms were located in a difference map, but were refined with fixed individual displacement parameters [U_{iso}(H) = 1.2 U_{eq}(C,*P*) using a riding model with C—H = 0.95 Å. In addition the P—H bond length [1.3486 Å] was refined (AFIX 14 option in *SHELXL97*).

Figures



Perspective view of the two molecules of the title compound with the atom numbering scheme; displacement ellipsoids are at the 50% probability level. H atoms are drawn as small spheres of arbitrary radii.
Partial packing diagram of the title compound. H atoms bonded to C have been omitted. Hydrogen bonds are shown as dashed lines.



Diphenylphosphane selenide

Crystal data

$C_{12}H_{11}PSe$	F_{000} = 1056
M_r = 265.14	D_x = 1.563 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 32153 reflections
a = 6.0901 (3) Å	θ = 2.0–26.0º
b = 32.3775 (18) Å	μ = 3.43 mm^{-1}
c = 11.5057 (6) Å	T = 173 (2) K
β = 96.741 (4)º	Rod, colourless
V = 2253.0 (2) Å^3	0.39 × 0.22 × 0.18 mm
Z = 8	

Data collection

Stoe IPDSII two-circle diffractometer	4221 independent reflections
Radiation source: fine-focus sealed tube	3625 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.071
T = 173(2) K	θ_{max} = 25.6º
ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	h = −7→7
T_{min} = 0.348, T_{max} = 0.577	k = −39→39
31769 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
$R[F^2 > 2\sigma(F^2)]$ = 0.041	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.107	$w = 1/[\sigma^2(F_o^2) + (0.0645P)^2 + 0.5807P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
4221 reflections	$\Delta\rho_{max}$ = 0.60 e Å^{-3}
255 parameters	$\Delta\rho_{min}$ = −0.82 e Å^{-3}

Primary atom site location: structure-invariant direct methods

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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}
P1	0.09835 (13)	0.33963 (3)	0.69820 (7)	0.03192 (19)
H1	−0.047 (4)	0.34283 (9)	0.778 (2)	0.038*
Se1	0.41802 (5)	0.342757 (11)	0.79157 (3)	0.03972 (13)
C1	0.0409 (5)	0.38172 (10)	0.5955 (3)	0.0350 (7)
C2	−0.1574 (6)	0.40311 (11)	0.5927 (4)	0.0474 (9)
H2	−0.2620	0.3957	0.6442	0.057*
C3	−0.2018 (8)	0.43557 (13)	0.5136 (4)	0.0593 (11)
H3	−0.3369	0.4504	0.5118	0.071*
C4	−0.0525 (8)	0.44628 (13)	0.4389 (4)	0.0594 (11)
H4	−0.0839	0.4685	0.3856	0.071*
C5	0.1453 (7)	0.42461 (14)	0.4409 (4)	0.0593 (11)
H5	0.2482	0.4317	0.3883	0.071*
C6	0.1913 (6)	0.39280 (12)	0.5196 (3)	0.0485 (9)
H6	0.3275	0.3783	0.5218	0.058*
C11	0.0369 (5)	0.29206 (9)	0.6194 (3)	0.0322 (6)
C12	0.1862 (6)	0.27636 (11)	0.5477 (3)	0.0401 (7)
H12	0.3223	0.2902	0.5427	0.048*
C13	0.1371 (6)	0.24062 (11)	0.4838 (3)	0.0459 (8)
H13	0.2381	0.2302	0.4341	0.055*
C14	−0.0590 (6)	0.22023 (11)	0.4927 (3)	0.0466 (9)
H14	−0.0922	0.1956	0.4492	0.056*
C15	−0.2081 (6)	0.23531 (11)	0.5645 (3)	0.0444 (8)
H15	−0.3427	0.2210	0.5701	0.053*
C16	−0.1609 (5)	0.27127 (10)	0.6284 (3)	0.0394 (7)
H16	−0.2627	0.2816	0.6778	0.047*
P1A	0.62143 (12)	0.40880 (2)	0.04919 (7)	0.03085 (19)
H1A	0.450 (4)	0.40567 (8)	−0.032 (2)	0.037*
Se1A	0.90789 (5)	0.403223 (11)	−0.03664 (3)	0.03914 (13)
C1A	0.5929 (5)	0.36893 (10)	0.1560 (3)	0.0317 (6)
C2A	0.3935 (6)	0.34771 (11)	0.1572 (3)	0.0395 (8)
H2A	0.2705	0.3545	0.1019	0.047*

C3A	0.3743 (6)	0.31662 (12)	0.2392 (4)	0.0481 (9)
H3A	0.2386	0.3022	0.2397	0.058*
C4A	0.5534 (6)	0.30689 (12)	0.3198 (3)	0.0485 (9)
H4A	0.5413	0.2855	0.3751	0.058*
C5A	0.7517 (7)	0.32840 (13)	0.3200 (3)	0.0496 (9)
H5A	0.8736	0.3218	0.3762	0.059*
C6A	0.7721 (6)	0.35908 (12)	0.2394 (3)	0.0416 (8)
H6A	0.9078	0.3736	0.2402	0.050*
C11A	0.5967 (5)	0.45790 (10)	0.1226 (3)	0.0313 (6)
C12A	0.7636 (5)	0.48738 (11)	0.1288 (3)	0.0379 (7)
H12A	0.8942	0.4823	0.0933	0.045*
C13A	0.7382 (6)	0.52438 (10)	0.1875 (3)	0.0415 (8)
H13A	0.8526	0.5445	0.1923	0.050*
C14A	0.5483 (6)	0.53210 (11)	0.2387 (3)	0.0433 (8)
H14A	0.5326	0.5573	0.2790	0.052*
C15A	0.3807 (6)	0.50289 (11)	0.2312 (3)	0.0453 (8)
H15A	0.2490	0.5084	0.2653	0.054*
C16A	0.4043 (5)	0.46583 (11)	0.1742 (3)	0.0397 (7)
H16A	0.2898	0.4458	0.1702	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0343 (4)	0.0320 (4)	0.0296 (4)	−0.0020 (3)	0.0044 (3)	−0.0027 (3)
Se1	0.0381 (2)	0.0440 (2)	0.0356 (2)	−0.00395 (13)	−0.00179 (14)	−0.00289 (14)
C1	0.0412 (16)	0.0327 (16)	0.0304 (17)	−0.0033 (13)	0.0010 (13)	−0.0015 (13)
C2	0.049 (2)	0.045 (2)	0.048 (2)	0.0050 (16)	0.0043 (17)	0.0004 (16)
C3	0.067 (3)	0.046 (2)	0.062 (3)	0.0133 (19)	−0.006 (2)	0.0061 (19)
C4	0.085 (3)	0.045 (2)	0.044 (2)	−0.006 (2)	−0.013 (2)	0.0096 (17)
C5	0.067 (3)	0.067 (3)	0.043 (2)	−0.017 (2)	0.0028 (19)	0.0141 (19)
C6	0.048 (2)	0.049 (2)	0.048 (2)	−0.0063 (17)	0.0035 (17)	0.0046 (17)
C11	0.0348 (15)	0.0297 (15)	0.0316 (16)	−0.0012 (12)	0.0023 (12)	−0.0004 (12)
C12	0.0363 (16)	0.0416 (18)	0.043 (2)	−0.0017 (14)	0.0072 (14)	−0.0047 (15)
C13	0.050 (2)	0.043 (2)	0.045 (2)	0.0052 (16)	0.0070 (16)	−0.0130 (16)
C14	0.063 (2)	0.0311 (17)	0.043 (2)	−0.0027 (16)	−0.0056 (17)	−0.0049 (15)
C15	0.0415 (18)	0.0385 (18)	0.051 (2)	−0.0077 (14)	−0.0028 (16)	0.0022 (16)
C16	0.0345 (16)	0.0392 (18)	0.044 (2)	−0.0009 (13)	0.0041 (14)	−0.0005 (15)
P1A	0.0289 (4)	0.0327 (4)	0.0303 (4)	0.0010 (3)	0.0006 (3)	−0.0005 (3)
Se1A	0.0353 (2)	0.0450 (2)	0.0380 (2)	0.00360 (13)	0.00777 (14)	0.00016 (14)
C1A	0.0341 (15)	0.0314 (16)	0.0292 (16)	0.0021 (12)	0.0021 (12)	−0.0008 (12)
C2A	0.0345 (16)	0.0426 (19)	0.041 (2)	0.0030 (14)	0.0044 (14)	0.0026 (14)
C3A	0.0429 (18)	0.048 (2)	0.055 (2)	0.0011 (16)	0.0121 (16)	0.0112 (17)
C4A	0.055 (2)	0.051 (2)	0.041 (2)	0.0041 (17)	0.0118 (16)	0.0115 (16)
C5A	0.058 (2)	0.055 (2)	0.0336 (19)	0.0100 (18)	−0.0036 (16)	0.0056 (16)
C6A	0.0403 (18)	0.045 (2)	0.0378 (19)	−0.0002 (14)	−0.0026 (14)	−0.0015 (15)
C11A	0.0324 (15)	0.0321 (16)	0.0285 (16)	0.0020 (12)	0.0003 (12)	0.0019 (12)
C12A	0.0335 (16)	0.0408 (18)	0.0397 (19)	−0.0030 (13)	0.0060 (13)	0.0019 (14)
C13A	0.0419 (18)	0.0347 (17)	0.047 (2)	−0.0068 (14)	0.0017 (15)	0.0029 (15)

C14A	0.053 (2)	0.0322 (17)	0.044 (2)	0.0031 (15)	0.0042 (16)	−0.0043 (14)
C15A	0.0408 (18)	0.044 (2)	0.053 (2)	0.0030 (15)	0.0130 (16)	−0.0077 (17)
C16A	0.0335 (16)	0.0383 (18)	0.048 (2)	−0.0031 (13)	0.0084 (14)	−0.0030 (15)

Geometric parameters (Å, °)

P1—C11	1.804 (3)	P1A—C1A	1.804 (3)
P1—C1	1.810 (3)	P1A—C11A	1.815 (3)
P1—Se1	2.1127 (9)	P1A—Se1A	2.1109 (9)
P1—H1	1.3486	P1A—H1A	1.3164
C1—C6	1.385 (5)	C1A—C2A	1.397 (5)
C1—C2	1.389 (5)	C1A—C6A	1.403 (4)
C2—C3	1.395 (5)	C2A—C3A	1.394 (5)
C2—H2	0.9500	C2A—H2A	0.9500
C3—C4	1.367 (7)	C3A—C4A	1.383 (5)
C3—H3	0.9500	C3A—H3A	0.9500
C4—C5	1.392 (7)	C4A—C5A	1.394 (6)
C4—H4	0.9500	C4A—H4A	0.9500
C5—C6	1.378 (6)	C5A—C6A	1.374 (5)
C5—H5	0.9500	C5A—H5A	0.9500
C6—H6	0.9500	C6A—H6A	0.9500
C11—C12	1.393 (5)	C11A—C12A	1.390 (4)
C11—C16	1.395 (4)	C11A—C16A	1.399 (5)
C12—C13	1.385 (5)	C12A—C13A	1.392 (5)
C12—H12	0.9500	C12A—H12A	0.9500
C13—C14	1.379 (5)	C13A—C14A	1.382 (5)
C13—H13	0.9500	C13A—H13A	0.9500
C14—C15	1.386 (5)	C14A—C15A	1.387 (5)
C14—H14	0.9500	C14A—H14A	0.9500
C15—C16	1.388 (5)	C15A—C16A	1.383 (5)
C15—H15	0.9500	C15A—H15A	0.9500
C16—H16	0.9500	C16A—H16A	0.9500
C11—P1—C1	107.56 (14)	C1A—P1A—C11A	106.86 (14)
C11—P1—Se1	114.89 (10)	C1A—P1A—Se1A	114.09 (10)
C1—P1—Se1	113.06 (11)	C11A—P1A—Se1A	114.26 (10)
C11—P1—H1	107.0	C1A—P1A—H1A	107.1
C1—P1—H1	107.0	C11A—P1A—H1A	107.1
Se1—P1—H1	107.0	Se1A—P1A—H1A	107.1
C6—C1—C2	119.6 (3)	C2A—C1A—C6A	119.3 (3)
C6—C1—P1	121.0 (3)	C2A—C1A—P1A	120.8 (2)
C2—C1—P1	119.4 (3)	C6A—C1A—P1A	119.9 (3)
C1—C2—C3	119.5 (4)	C3A—C2A—C1A	120.3 (3)
C1—C2—H2	120.3	C3A—C2A—H2A	119.9
C3—C2—H2	120.3	C1A—C2A—H2A	119.9
C4—C3—C2	120.6 (4)	C4A—C3A—C2A	119.7 (3)
C4—C3—H3	119.7	C4A—C3A—H3A	120.1
C2—C3—H3	119.7	C2A—C3A—H3A	120.1
C3—C4—C5	120.0 (4)	C3A—C4A—C5A	120.2 (3)
C3—C4—H4	120.0	C3A—C4A—H4A	119.9

C5—C4—H4	120.0	C5A—C4A—H4A	119.9
C6—C5—C4	119.8 (4)	C6A—C5A—C4A	120.4 (3)
C6—C5—H5	120.1	C6A—C5A—H5A	119.8
C4—C5—H5	120.1	C4A—C5A—H5A	119.8
C5—C6—C1	120.6 (4)	C5A—C6A—C1A	120.1 (3)
C5—C6—H6	119.7	C5A—C6A—H6A	120.0
C1—C6—H6	119.7	C1A—C6A—H6A	120.0
C12—C11—C16	119.8 (3)	C12A—C11A—C16A	119.7 (3)
C12—C11—P1	119.8 (2)	C12A—C11A—P1A	121.7 (2)
C16—C11—P1	120.3 (2)	C16A—C11A—P1A	118.6 (2)
C13—C12—C11	120.2 (3)	C11A—C12A—C13A	119.6 (3)
C13—C12—H12	119.9	C11A—C12A—H12A	120.2
C11—C12—H12	119.9	C13A—C12A—H12A	120.2
C14—C13—C12	119.7 (3)	C14A—C13A—C12A	120.6 (3)
C14—C13—H13	120.1	C14A—C13A—H13A	119.7
C12—C13—H13	120.1	C12A—C13A—H13A	119.7
C13—C14—C15	120.6 (3)	C13A—C14A—C15A	119.8 (3)
C13—C14—H14	119.7	C13A—C14A—H14A	120.1
C15—C14—H14	119.7	C15A—C14A—H14A	120.1
C14—C15—C16	120.1 (3)	C16A—C15A—C14A	120.3 (3)
C14—C15—H15	120.0	C16A—C15A—H15A	119.8
C16—C15—H15	120.0	C14A—C15A—H15A	119.8
C15—C16—C11	119.5 (3)	C15A—C16A—C11A	120.0 (3)
C15—C16—H16	120.2	C15A—C16A—H16A	120.0
C11—C16—H16	120.2	C11A—C16A—H16A	120.0
C11—P1—C1—C6	−80.3 (3)	C11A—P1A—C1A—C2A	101.1 (3)
Se1—P1—C1—C6	47.6 (3)	Se1A—P1A—C1A—C2A	−131.6 (2)
C11—P1—C1—C2	99.5 (3)	C11A—P1A—C1A—C6A	−78.6 (3)
Se1—P1—C1—C2	−132.6 (3)	Se1A—P1A—C1A—C6A	48.7 (3)
C6—C1—C2—C3	−0.2 (5)	C6A—C1A—C2A—C3A	−1.1 (5)
P1—C1—C2—C3	179.9 (3)	P1A—C1A—C2A—C3A	179.2 (3)
C1—C2—C3—C4	0.4 (6)	C1A—C2A—C3A—C4A	0.2 (6)
C2—C3—C4—C5	0.2 (7)	C2A—C3A—C4A—C5A	0.8 (6)
C3—C4—C5—C6	−0.9 (7)	C3A—C4A—C5A—C6A	−0.8 (6)
C4—C5—C6—C1	1.1 (6)	C4A—C5A—C6A—C1A	−0.1 (6)
C2—C1—C6—C5	−0.5 (6)	C2A—C1A—C6A—C5A	1.0 (5)
P1—C1—C6—C5	179.3 (3)	P1A—C1A—C6A—C5A	−179.3 (3)
C1—P1—C11—C12	78.0 (3)	C1A—P1A—C11A—C12A	122.0 (3)
Se1—P1—C11—C12	−48.9 (3)	Se1A—P1A—C11A—C12A	−5.2 (3)
C1—P1—C11—C16	−101.0 (3)	C1A—P1A—C11A—C16A	−57.7 (3)
Se1—P1—C11—C16	132.2 (2)	Se1A—P1A—C11A—C16A	175.1 (2)
C16—C11—C12—C13	1.2 (5)	C16A—C11A—C12A—C13A	0.6 (5)
P1—C11—C12—C13	−177.8 (3)	P1A—C11A—C12A—C13A	−179.1 (3)
C11—C12—C13—C14	−1.0 (5)	C11A—C12A—C13A—C14A	−0.4 (5)
C12—C13—C14—C15	0.4 (6)	C12A—C13A—C14A—C15A	−0.4 (6)
C13—C14—C15—C16	0.0 (6)	C13A—C14A—C15A—C16A	1.0 (6)
C14—C15—C16—C11	0.2 (5)	C14A—C15A—C16A—C11A	−0.8 (6)
C12—C11—C16—C15	−0.8 (5)	C12A—C11A—C16A—C15A	0.0 (5)
P1—C11—C16—C15	178.2 (3)	P1A—C11A—C16A—C15A	179.8 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
P1A—H1A···Se1^{i}	1.32	2.87	3.7458 (9)	123
P1—H1···Se1A^{ii}	1.35	2.93	3.9652 (9)	132

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) *x*−1, *y*, *z*+1.

Fig. 1

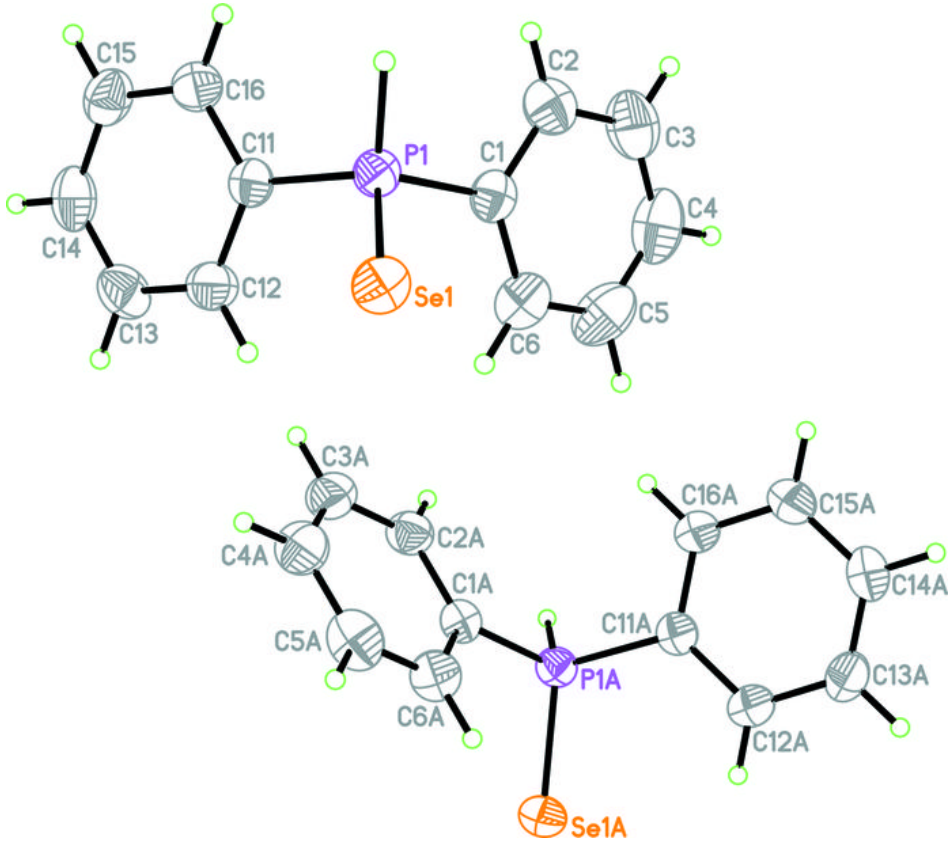

C15
C16
C11
P1
C1
C2
C3
C4
C14
C12
Se1
C5
C13
C6
C3A
C16A
C15A
C2A
C4A
C1A
C14A
C11A
C5A
P1A
C13A
C6A
C12A
Se1A

Fig. 2

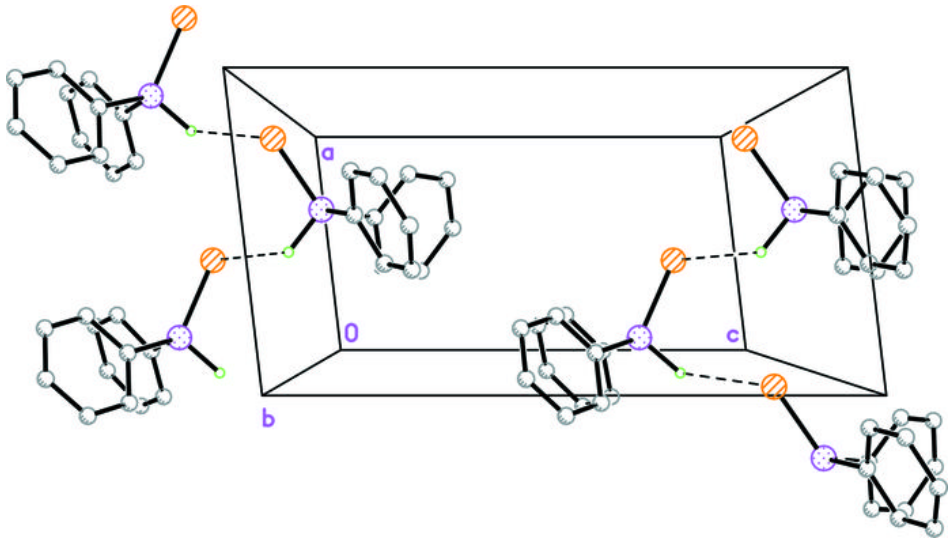


Fig. 3