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Benzyldiphenylphosphine selenide

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In the molecule of the title compound, SePPh$_2$Bz (Bz = benzyl, CH$_2$C$_6$H$_5$) or C$_{19}$H$_{17}$PSe, the Se atom and the three aryl groups adopt a distorted tetrahedral arrangement about the P atom. The effective cone angle was calculated to be 167°.

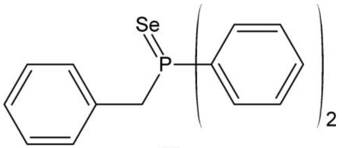
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.030
wR factor = 0.063
Data-to-parameter ratio = 17.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

There has been extensive development in understanding the transition metal–phosphorus bond by various groups, including our own (Roodt *et al.*, 2003), with various techniques such as single-crystal X-ray crystallography, multi-nuclear NMR and IR spectroscopy. As part of this systematic investigation, we are now also studying selenium derivatives of phosphorus ligands. In this approach there is no steric crowding effect, though there remain crystal packing effects, as normally found in transition metal complexes with bulky ligands, *e.g.* in *trans*-[Rh(CO)Cl{P(OC$_6$H$_5$)$_3$}$_2$] cone-angle variation from 156° to 167° was observed for the two phosphite ligands (Muller *et al.*, 2006). $^1J(^{31}\mathrm{P}–^{77}\mathrm{Se})$ coupling can also be used as an additional probe to obtain more information regarding the nature of the phosphorus–selenium bond. We report here the structure of the selenium derivative of the unsymmetrical phosphine PPh$_2$Bz.



(I)

All features of the title molecule, (I), are as expected [Cambridge Structural Database (CSD), Version 5.27, August

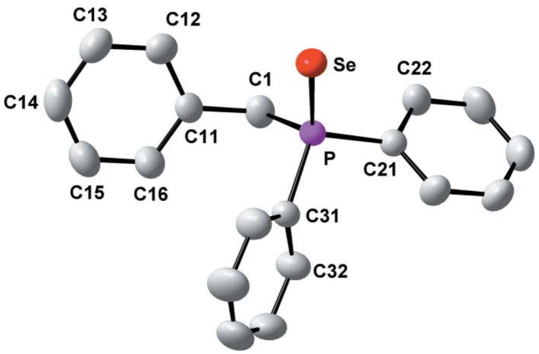


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity. For the aromatic C atoms, the first digit indicates the ring number and the second digit indicates the position of the atom in the ring.

2006 update; Allen, 2002], with the Se atom and the three aryl groups adopting a distorted tetrahedral arrangement about the P atom (Fig. 1 and Table 1).

The cone angle was calculated as described previously (Tolman, 1977 and Otto *et al.*, 2000), with the Se atom repositioned to 2.28 Å from the P atom. A value of 167° was obtained for (I), which is comparable to those in metal–PPh_2Bz complexes we have reported previously (Meijboom *et al.*, 2006*a*,*b*). It is noted that the benzyl substituent can adopt two distinct orientations, showing the ability of the ligand to adjust for the effect of steric crowding in the metal environment. Transition metal complexes with the benzyl group pointing toward the metal center have a cone angle value of ~161°, while ~141° is observed if the benzyl group is pointing away (data extracted and calculated from 18 examples in the CSD).

Experimental

PPh_2Bz and KSeCN were bought from Sigma–Aldrich and used as received. Eqimolar amounts of KSeCN and PPh_2Bz (*ca* 0.04 mmol) were each dissolved in minimum amounts of methanol (10–20 ml). The KSeCN solution was added dropwise over 5 min to the phosphine solution with stirring at room temperature. The final solution was left to evaporate slowly until dry, giving crystals suitable for X-ray analysis. $^{31}P\{H\}NMR$ ($CDCl_3$, 121.42 MHz): δ 35.2 (*t*, $^1J_{(P-Se)}$ = 735 Hz).

Crystal data

$C_{19}H_{17}PSe$
$M_r = 355.26$
Orthorhombic, $Pna2_1$
$a = 10.572$ (2) Å
$b = 9.789$ (2) Å
$c = 16.009$ (3) Å
$V = 1656.8$ (6) Å^3
$Z = 4$
$D_x = 1.424$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 2.35$ mm^{-1}
$T = 294$ (2) K
Block, colorless
0.36 × 0.3 × 0.2 mm

Data collection

Bruker SMART CCD 1K diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.465$, $T_{max} = 0.624$
6219 measured reflections
3343 independent reflections
2766 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 28.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.03$
$wR(F^2) = 0.063$
$S = 1$
3343 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.011P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Absolute structure: Flack (1983), with 1216 Friedel pairs
Flack parameter: 0.025 (9)

Table 1
Selected geometric parameters (Å, °).

Se—P	2.1117 (8)	P—C31	1.817 (3)
P—C21	1.815 (3)	P—C1	1.836 (3)
C21—P—C31	106.00 (13)	C21—P—Se	111.69 (9)
C21—P—C1	105.48 (12)	C31—P—Se	115.00 (9)
C31—P—C1	104.35 (14)	C1—P—Se	113.49 (11)

H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 1999); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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