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2-Isobutyl-2-phosphabicyclo[3.3.1]-nonane 2-selenide

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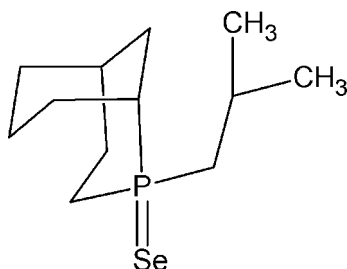
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.010$ Å; R factor = 0.059; wR factor = 0.181; data-to-parameter ratio = 26.1.

The title compound, $\text{C}_{12}\text{H}_{23}\text{PSe}$, represents the first structure of a phosphine containing the bicyclic 2-phosphabicyclo[3.3.1]nonane (VCH) unit. It contains two chiral centres per molecule which can be either R,R - or S,S and crystallizes as a centrosymmetric, racemic mixture of the enantiomers. The P—Se bond distance of 2.1360 (16) Å is typical for these compounds. The Tolman cone angle (2.28 Å from P) was calculated as 163°, and the effective cone angle (using the crystallographically determined P—Se bond distance) is 168°.

Related literature

For the synthesis of phosphine selenides, see: Otto *et al.* (2005). For the evaluation of ligand electronic properties, see: Allen & Taylor (1982); Bungu & Otto (2007b); Muller *et al.* (2008); Otto & Roodt (2004); Roodt & Steyn (2000). For the application of bicyclic ligands in catalysis, see: Bungu & Otto (2007a); Crause *et al.* (2003); Dwyer *et al.* (2004); Steynberg *et al.* (2003); Van Winkle *et al.* (1969). For information on cone angles, see: Tolman (1977); Otto (2001).



Experimental

Crystal data

$\text{C}_{12}\text{H}_{23}\text{PSe}$
 $M_r = 277.23$
 Monoclinic, $P2_1/c$

$a = 10.763$ (2) Å
 $b = 7.2540$ (15) Å
 $c = 17.530$ (4) Å

$\beta = 97.93$ (3)°
 $V = 1355.6$ (5) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 2.85$ mm⁻¹
 $T = 293$ K
 $0.14 \times 0.12 \times 0.08$ mm

Data collection

Bruker X8 APEXII 4K KappaCCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2008)
 $T_{\min} = 0.691$, $T_{\max} = 0.804$

9132 measured reflections
 3366 independent reflections
 1658 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.062$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.059$
 $wR(F^2) = 0.181$
 $S = 1.02$
 3366 reflections

129 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.58$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.58$ e Å⁻³

Table 1

X-ray and spectroscopic data (Å, Hz) for selected phosphine selenides.

P	Se—P	¹ J _{Se—P}
PMe ₃ ⁱ	2.111 (3)	684
PCy ₃ ⁱⁱ	2.108 (1)	676
VCH- ^t Bu ⁱⁱⁱ	2.1360 (16)	672, 687
Phoban-Ph ^{iv}	2.1090 (9)	689, 717
PPhCy ₂ ^v	2.1260 (8)	701
P(<i>o</i> -Tol) ₃ ^{vi}	2.116 (5)	708
PPh ₂ Cy ^v	2.111 (2)	725
PPh ₃ ^{vii}	2.106 (1)	733
P(NMe ₂) ₃ ^{viii}	2.120 (1)	797

Notes: (i) Cogne *et al.* (1980); (ii) Davies *et al.* (1991); (iii) this work; (iv) Bungu & Otto (2007b); (v) Muller *et al.* (2008); (vi) Cameron & Dahlen (1975); (vii) Codding & Kerr (1979); (viii) Rømming & Songstad (1979).

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT-Plus (Bruker, 2004); data reduction: SAINT-Plus and XPREP (Bruker, 2004); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg & Berndt, 2001); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2909).

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supporting information

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2-Isobutyl-2-phosphabicyclo[3.3.1]nonane 2-selenide

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S1. Comment

It is well established that the steric and electronic properties of phosphine ligands have a major influence on the chemistry of its metal species. Several methods are used to quantify the electronic characteristics of phosphines, including NMR measurements of first order Pt—P, Rh—P, Se—P and P—BH₃ coupling constants (Allen & Taylor, 1982 and Roodt & Steyn, 2000) and measuring of CO stretching frequencies in complexes such as [Ni(L)(CO)₃] (Tolman, 1977) or *trans*-[RhCl(CO)(L)₂] (Otto & Roodt, 2004).

Phosphine ligands containing bicyclic substituents have been shown to add significant benefits to the catalytic performance of several homogeneously catalysed systems (Bungu & Otto, 2007a). The best known example is the 9-phosphabicyclo[3.3.1]nonane and 9-phosphabicyclo[4.2.1]nonane mixture of isomers (Phoban family of ligands) patented by Shell (Van Winkle *et al.*, 1969) for modified cobalt hydroformylation. Sasol has reported on the use of bicyclic phosphines derived from (*R*)-(+)-Limonene (Lim family) (Crause *et al.*, 2003, Dwyer *et al.*, 2004) and vinylcyclohexene (VCH family) (Steynberg *et al.*, 2003) for similar applications.

After a convenient synthetic protocol for phosphine selenides were developed (Otto *et al.*, 2005) we extensively used the Se—P coupling constants for the quantification of electronic properties of phosphine ligands (Bungu & Otto, 2007b). Smaller values for the coupling constants correspond with ligands of higher basicity (more electron donating). We now report the synthesis and crystallographic characterization of the title compound, (I), 2-isobutyl-2-phosphabicyclo[3.3.1]nonane 2-selenide (VCH-ⁱBu) which represents the first crystal structure of a VCH family member.

Compound (I) crystallizes in the monoclinic space group P2/c and consists of the VCH backbone, the iso-butyl side chain and the selenium atom coordinated to phosphorus in a tetrahedral fashion. The compound contains two chiral centres on the VCH backbone (C13 and C15) which can be *R,R*- or *S,S* (as in the arbitrarily chosen asymmetric molecule; Fig. 1) and it crystallizes as a racemic mixture on account of the centrosymmetric space group. The P atom could also be considered as chiral based on the four different substituents. All bond distances and angles are within normal ranges. Even though larger Se—P coupling constants are indicative of more effective s-orbital overlap no clear trends are evident in the Se—P bond distances.

The packing in the unit cell is governed by van der Waals forces alone since no pertinent intramolecular interactions were evident. The Tolman- (2.28 Å from P) and effective cone angles (using the crystallographically determined Se—P bond distance) were calculated (Otto, 2001) resulting in values of 163 and 168° respectively.

S2. Experimental

2-Isobutyl-2-phosphabicyclo[3.3.1]nonane was generously supplied by Cytec; it exists as two stereo isomers in close to equal quantities. ³¹P (CDCl₃): -36.23 and -35.22 p.p.m..

The title compound was prepared according to the procedure described previously (Bungu & Otto, 2007b), colourless blocks of (I) were obtained by evaporation of a dichloromethane solution. ³¹P (CDCl₃): 29.72 p.p.m. (¹J_{Se-P} = 684 Hz) and

29.88 p.p.m. ($^1J_{\text{Se-P}} = 670$ Hz).

S3. Refinement

The H atoms were placed in geometrically idealized positions (CH = 0.98, CH₂ = 0.97 and CH₃ = 0.96 Å) and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for CH and CH₂ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for CH₃.

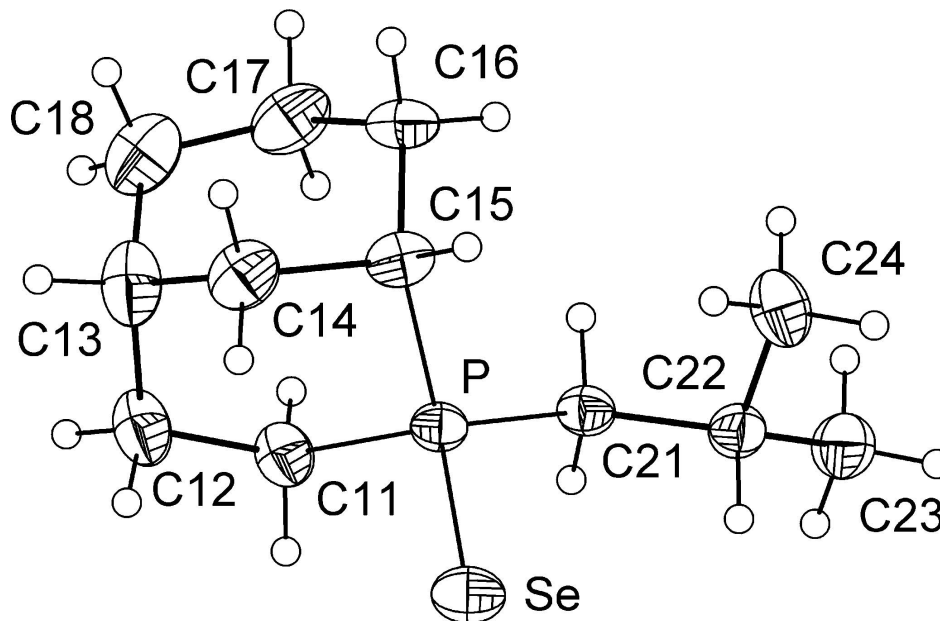


Figure 1

Molecular diagram of (I) showing 30% displacement ellipsoids.

2-Isobutyl-2-phosfabicyclo[3.3.1]nonane 2-selenide

Crystal data

C₁₂H₂₃PSe

$M_r = 277.23$

Monoclinic, *P2/c*

$a = 10.763$ (2) Å

$b = 7.2540$ (15) Å

$c = 17.530$ (4) Å

$\beta = 97.93$ (3)°

$V = 1355.6$ (5) Å³

$Z = 4$

$F(000) = 576$

$D_x = 1.358$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1002 reflections

$\theta = 2.8$ – 25.7 °

$\mu = 2.85$ mm⁻¹

$T = 293$ K

Block, colourless

$0.14 \times 0.12 \times 0.08$ mm

Data collection

Bruker X8 APEXII 4K KappaCCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 512 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2008)

$T_{\text{min}} = 0.691$, $T_{\text{max}} = 0.804$

9132 measured reflections

3366 independent reflections

1658 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.062$

$\theta_{\text{max}} = 28.3$ °, $\theta_{\text{min}} = 1.9$ °

$h = -11 \rightarrow 14$

$k = -8 \rightarrow 9$

$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.059$
 $wR(F^2) = 0.181$
 $S = 1.02$
 3366 reflections
 129 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0816P)^2 + 0.9034P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.58 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.58 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. The intensity data were collected on a Bruker X8 ApexII 4 K Kappa CCD diffractometer using an exposure time of 40 s/frame with a frame width of 0.3°; a total of 1315 frames were collected.

The crystals were of poor quality and were, as a precautionary measure, covered with Canada balsam. Consequently some intensity in the reflexions were sacrificed and the completeness is somewhat low at high angles.

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 $F^2 > \sigma(F^2)$ 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>	$U_{\text{iso}}^*/U_{\text{eq}}$
P	0.21847 (13)	-0.0934 (2)	-0.03355 (8)	0.0418 (4)
Se	0.23308 (6)	0.16679 (9)	0.02405 (4)	0.0633 (3)
C11	0.1179 (6)	-0.0851 (9)	-0.1269 (3)	0.0588 (16)
H11A	0.0957	-0.2100	-0.1433	0.071*
H11B	0.0410	-0.0206	-0.1207	0.071*
C12	0.1797 (6)	0.0105 (11)	-0.1899 (4)	0.0712 (19)
H12A	0.1870	0.1411	-0.1780	0.085*
H12B	0.1251	-0.0022	-0.2384	0.085*
C13	0.3099 (7)	-0.0640 (12)	-0.1997 (4)	0.078 (2)
H13	0.3411	0.0092	-0.2401	0.094*
C14	0.3999 (6)	-0.0340 (10)	-0.1255 (4)	0.0699 (19)
H14A	0.3940	0.0930	-0.1090	0.084*
H14B	0.4852	-0.0554	-0.1353	0.084*
C15	0.3697 (5)	-0.1675 (8)	-0.0582 (4)	0.0528 (15)
H15	0.4336	-0.1494	-0.0133	0.063*
C16	0.3785 (6)	-0.3676 (8)	-0.0870 (4)	0.0610 (17)
H16A	0.4652	-0.3938	-0.0924	0.073*
H16B	0.3544	-0.4505	-0.0481	0.073*
C17	0.2984 (7)	-0.4081 (11)	-0.1622 (4)	0.082 (2)
H17A	0.2112	-0.4131	-0.1538	0.099*
H17B	0.3208	-0.5285	-0.1802	0.099*

C18	0.3119 (8)	-0.2667 (14)	-0.2240 (5)	0.091 (2)
H18A	0.2446	-0.2859	-0.2661	0.110*
H18B	0.3903	-0.2900	-0.2438	0.110*
C21	0.1449 (5)	-0.2707 (7)	0.0190 (3)	0.0452 (13)
H21A	0.0547	-0.2558	0.0076	0.054*
H21B	0.1655	-0.3899	-0.0010	0.054*
C22	0.1795 (5)	-0.2755 (8)	0.1068 (3)	0.0490 (14)
H22	0.1706	-0.1505	0.1266	0.059*
C23	0.0893 (6)	-0.4026 (10)	0.1427 (4)	0.0680 (18)
H23A	0.0046	-0.3618	0.1277	0.102*
H23B	0.1087	-0.3991	0.1978	0.102*
H23C	0.0981	-0.5265	0.1250	0.102*
C24	0.3154 (6)	-0.3372 (10)	0.1303 (4)	0.0708 (19)
H24A	0.3258	-0.4603	0.1121	0.106*
H24B	0.3350	-0.3345	0.1854	0.106*
H24C	0.3707	-0.2554	0.1080	0.106*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P	0.0394 (8)	0.0373 (7)	0.0482 (8)	-0.0002 (6)	0.0044 (6)	-0.0054 (6)
Se	0.0709 (5)	0.0383 (4)	0.0804 (5)	-0.0015 (3)	0.0100 (3)	-0.0152 (3)
C11	0.056 (4)	0.061 (4)	0.057 (4)	0.000 (3)	0.002 (3)	0.007 (3)
C12	0.062 (4)	0.085 (5)	0.063 (4)	-0.003 (4)	-0.001 (3)	0.022 (4)
C13	0.067 (5)	0.105 (7)	0.060 (4)	-0.018 (4)	0.001 (3)	0.017 (4)
C14	0.062 (4)	0.074 (5)	0.077 (5)	-0.013 (3)	0.020 (4)	-0.006 (4)
C15	0.039 (3)	0.054 (4)	0.065 (4)	-0.005 (3)	0.006 (3)	-0.014 (3)
C16	0.055 (4)	0.047 (4)	0.083 (5)	0.008 (3)	0.018 (3)	-0.010 (3)
C17	0.091 (6)	0.080 (5)	0.078 (5)	-0.010 (4)	0.019 (4)	-0.032 (4)
C18	0.093 (6)	0.108 (7)	0.075 (5)	-0.014 (5)	0.020 (4)	-0.018 (5)
C21	0.047 (3)	0.036 (3)	0.052 (3)	0.001 (2)	0.008 (3)	-0.003 (2)
C22	0.056 (4)	0.042 (3)	0.049 (3)	0.000 (3)	0.009 (3)	-0.004 (3)
C23	0.073 (5)	0.063 (4)	0.073 (4)	-0.001 (4)	0.027 (4)	0.010 (3)
C24	0.068 (4)	0.078 (5)	0.062 (4)	-0.008 (4)	-0.009 (3)	0.013 (4)

Geometric parameters (Å, °)

P—C15	1.822 (6)	C16—H16A	0.9700
P—C21	1.825 (6)	C16—H16B	0.9700
P—C11	1.835 (6)	C17—C18	1.514 (12)
P—Se	2.1360 (16)	C17—H17A	0.9700
C11—C12	1.531 (9)	C17—H17B	0.9700
C11—H11A	0.9700	C18—H18A	0.9700
C11—H11B	0.9700	C18—H18B	0.9700
C12—C13	1.534 (10)	C21—C22	1.533 (8)
C12—H12A	0.9700	C21—H21A	0.9700
C12—H12B	0.9700	C21—H21B	0.9700
C13—C14	1.527 (9)	C22—C24	1.530 (9)

C13—C18	1.532 (12)	C22—C23	1.536 (8)
C13—H13	0.9800	C22—H22	0.9800
C14—C15	1.594 (9)	C23—H23A	0.9600
C14—H14A	0.9700	C23—H23B	0.9600
C14—H14B	0.9700	C23—H23C	0.9600
C15—C16	1.544 (8)	C24—H24A	0.9600
C15—H15	0.9800	C24—H24B	0.9600
C16—C17	1.501 (9)	C24—H24C	0.9600
C15—P—C21	112.0 (3)	C17—C16—H16B	108.6
C15—P—C11	103.6 (3)	C15—C16—H16B	108.6
C21—P—C11	103.3 (3)	H16A—C16—H16B	107.6
C15—P—Se	111.27 (19)	C16—C17—C18	113.3 (6)
C21—P—Se	113.12 (19)	C16—C17—H17A	108.9
C11—P—Se	112.9 (2)	C18—C17—H17A	108.9
C12—C11—P	113.3 (4)	C16—C17—H17B	108.9
C12—C11—H11A	108.9	C18—C17—H17B	108.9
P—C11—H11A	108.9	H17A—C17—H17B	107.7
C12—C11—H11B	108.9	C17—C18—C13	116.4 (6)
P—C11—H11B	108.9	C17—C18—H18A	108.2
H11A—C11—H11B	107.7	C13—C18—H18A	108.2
C11—C12—C13	114.6 (6)	C17—C18—H18B	108.2
C11—C12—H12A	108.6	C13—C18—H18B	108.2
C13—C12—H12A	108.6	H18A—C18—H18B	107.3
C11—C12—H12B	108.6	C22—C21—P	117.4 (4)
C13—C12—H12B	108.6	C22—C21—H21A	107.9
H12A—C12—H12B	107.6	P—C21—H21A	107.9
C14—C13—C18	110.0 (7)	C22—C21—H21B	107.9
C14—C13—C12	109.6 (6)	P—C21—H21B	107.9
C18—C13—C12	114.7 (6)	H21A—C21—H21B	107.2
C14—C13—H13	107.4	C24—C22—C21	111.5 (5)
C18—C13—H13	107.4	C24—C22—C23	110.5 (5)
C12—C13—H13	107.4	C21—C22—C23	110.1 (5)
C13—C14—C15	112.0 (5)	C24—C22—H22	108.2
C13—C14—H14A	109.2	C21—C22—H22	108.2
C15—C14—H14A	109.2	C23—C22—H22	108.2
C13—C14—H14B	109.2	C22—C23—H23A	109.5
C15—C14—H14B	109.2	C22—C23—H23B	109.5
H14A—C14—H14B	107.9	H23A—C23—H23B	109.5
C16—C15—C14	107.5 (5)	C22—C23—H23C	109.5
C16—C15—P	116.8 (4)	H23A—C23—H23C	109.5
C14—C15—P	106.0 (4)	H23B—C23—H23C	109.5
C16—C15—H15	108.7	C22—C24—H24A	109.5
C14—C15—H15	108.7	C22—C24—H24B	109.5
P—C15—H15	108.7	H24A—C24—H24B	109.5
C17—C16—C15	114.7 (6)	C22—C24—H24C	109.5
C17—C16—H16A	108.6	H24A—C24—H24C	109.5
C15—C16—H16A	108.6	H24B—C24—H24C	109.5

C15—P—C11—C12	-45.9 (6)	C11—P—C15—C14	50.9 (4)
C21—P—C11—C12	-162.9 (5)	Se—P—C15—C14	-70.7 (4)
Se—P—C11—C12	74.6 (5)	C14—C15—C16—C17	-54.2 (7)
P—C11—C12—C13	52.2 (8)	P—C15—C16—C17	64.7 (7)
C11—C12—C13—C14	-62.0 (8)	C15—C16—C17—C18	48.6 (9)
C11—C12—C13—C18	62.3 (8)	C16—C17—C18—C13	-45.1 (10)
C18—C13—C14—C15	-55.5 (8)	C14—C13—C18—C17	48.8 (9)
C12—C13—C14—C15	71.5 (8)	C12—C13—C18—C17	-75.3 (8)
C13—C14—C15—C16	58.2 (7)	C15—P—C21—C22	87.0 (5)
C13—C14—C15—P	-67.5 (6)	C11—P—C21—C22	-162.1 (4)
C21—P—C15—C16	41.8 (6)	Se—P—C21—C22	-39.8 (5)
C11—P—C15—C16	-68.9 (5)	P—C21—C22—C24	-69.3 (6)
Se—P—C15—C16	169.6 (4)	P—C21—C22—C23	167.7 (4)
C21—P—C15—C14	161.6 (4)		
