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(*S*)-1-(Benzylselanyl)-3-phenylpropan-2-amine

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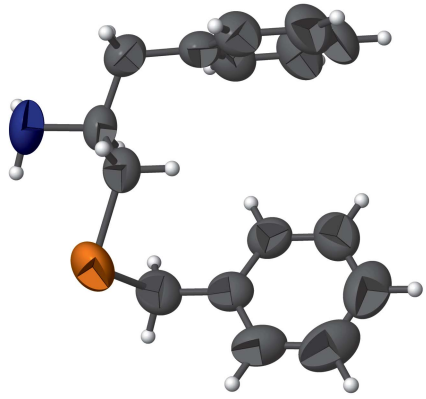
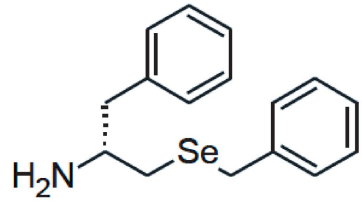
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{16}H_{19}NSe$, the dihedral angle between the benzene rings is 66.49 (12) and a weak intramolecular N—H···Se hydrogen bond generates an S(6) ring. In the crystal, weak N—H···N hydrogen bonds link the molecules into [100] chains.

3D view



Chemical scheme



Structure description

The title compound, $C_{16}H_{19}NSe$, is a chiral selenated amine that could act as a hybrid ligand of the (N,Se) type. This amine could further be used for the synthesis of chiral Schiff bases with various aldehydes/ketones, which may result in multidentate hybrid ligands (Kostas *et al.*, 2006; Kumar *et al.*, 2009).

The molecular structure is shown in Fig. 1. The dihedral angle between the benzene rings is 66.49 (12)° and the C7—Se1—C8—C9 torsion angle is 75.3 (5)°. A weak intramolecular N—H···Se hydrogen bond (Table 1) generates an *S*(5) ring. In the crystal, molecules are linked by weak N1—H2*N*···N1 interactions, generating [100] chains (Fig. 2).

Synthesis and crystallization

The title compound was synthesized according to our reported procedure (Rajegowda *et al.*, 2015). The light-yellow viscous liquid obtained was dissolved in a 1:1 mixture of dichloromethane and *n*-hexane, which was kept undisturbed in the refrigerator at 0°C. After four to five days, light-yellow crystals were collected by filtration and dried in air.

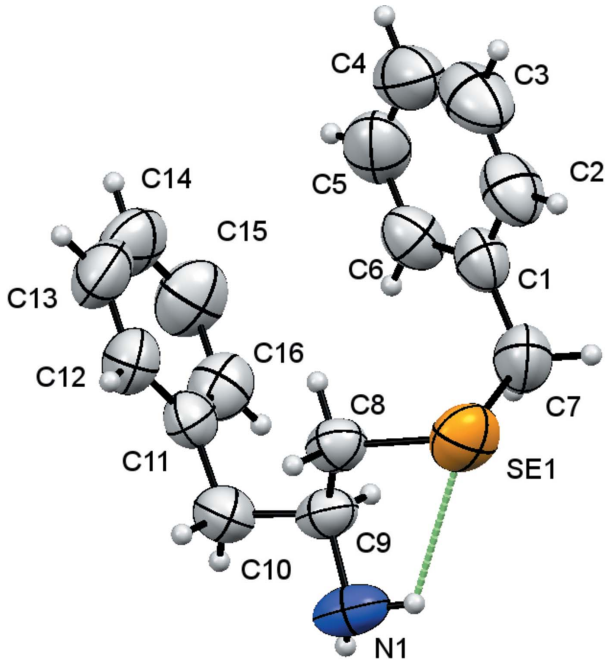


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

We are grateful to the facilities at BSPM Lab, Albert Einstein Block, University College of Science, Tumkur University, for the support related to crystallography work.

Funding information

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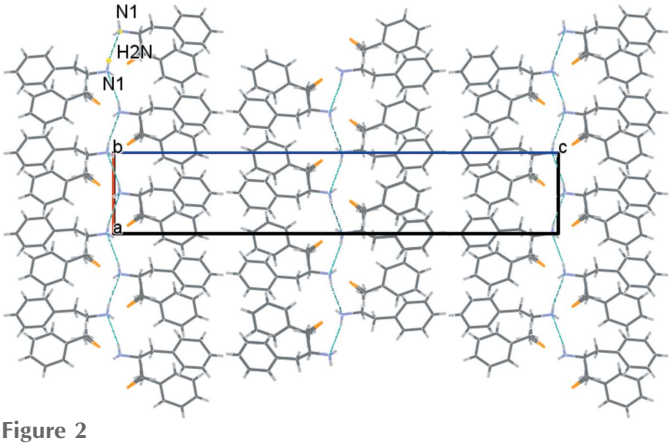

Figure 2
The packing of the title compound viewed along [010] showing the formation of [100] hydrogen-bonded chains.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···Se1	0.93 (7)	2.69 (7)	3.239 (7)	119 (5)
N1—H2*N*···N1^{i}	0.79 (5)	2.56 (5)	3.319 (5)	161 (4)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{19}NSe$
M_r	304.28
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	295
a, b, c (Å)	5.7670 (3), 8.1908 (3), 31.6737 (9)
V (Å^3)	1496.15 (10)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	3.24
Crystal size (mm)	0.32 × 0.28 × 0.22
Data collection	
Diffractometer	Rigaku Oxford Diffraction CCD
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.403, 0.490
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9030, 2848, 2501
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.616
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.122, 1.09
No. of reflections	2848
No. of parameters	171
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.39, −0.45
Absolute structure	Flack x determined using 861 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.015 (16)

Computer programs: *CrysAlis PRO* (Agilent, 2014, *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *Mercury* (Macrae *et al.*, 2008).

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full crystallographic data

IUCrData (2019). **4**, x191029 [https://doi.org/10.1107/S2414314619010290]

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Crystal data

$C_{16}H_{19}NSe$
M_r = 304.28
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 5.7670 (3) Å
b = 8.1908 (3) Å
c = 31.6737 (9) Å
V = 1496.15 (10) Å^3
Z = 4
$F(000)$ = 624
prism
D_x = 1.351 Mg m^{-3}
Melting point: 498 K
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 2501 reflections
θ = 1–71.8°
μ = 3.24 mm^{-1}
T = 295 K
Prism, yellow
0.32 × 0.28 × 0.22 mm

Data collection

Rigaku Oxford Diffraction CCD diffractometer
Radiation source: Cu Kα
Graphite monochromator
Detector resolution: 16.2 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.403, T_{max} = 0.490
9030 measured reflections
2848 independent reflections
2501 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 71.8°, θ_{min} = 5.6°
h = −7→6
k = −9→6
l = −37→38

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.122
S = 1.09
2848 reflections
171 parameters
0 restraints
3 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2 + 0.2035P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}
Absolute structure: Flack x determined using 861 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.015 (16)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The C-bound hydrogen atoms were fixed geometrically and allowed to ride on their parent atoms: C—H = 0.93–0.97Å. The N-bound H atoms were located in difference maps and their positions were freely refined. The constraint $U_{iso}(H) = 1.2U_{eq}$(carrier) was applied in all cases.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Se1	0.09270 (14)	0.59847 (9)	0.46926 (2)	0.0991 (3)
N1	0.4997 (11)	0.3335 (8)	0.48563 (15)	0.0909 (14)
H1N	0.447 (12)	0.424 (8)	0.501 (2)	0.10 (2)*
H2N	0.633 (9)	0.313 (6)	0.4892 (14)	0.051 (12)*
C1	0.1443 (9)	0.8034 (5)	0.39473 (16)	0.0771 (12)
C2	−0.0602 (10)	0.8816 (7)	0.3875 (2)	0.0964 (16)
H2A	−0.147323	0.919744	0.410166	0.116*
C3	−0.1392 (12)	0.9046 (9)	0.3468 (3)	0.116 (2)
H3A	−0.277636	0.959867	0.342064	0.139*
C4	−0.0145 (16)	0.8463 (8)	0.3137 (3)	0.113 (2)
H4A	−0.068275	0.861057	0.286291	0.135*
C5	0.1889 (15)	0.7662 (8)	0.3205 (2)	0.106 (2)
H5A	0.273920	0.726206	0.297845	0.127*
C6	0.2680 (10)	0.7449 (6)	0.36081 (18)	0.0823 (13)
H6A	0.407040	0.690101	0.365352	0.099*
C7	0.2370 (15)	0.7833 (7)	0.43881 (19)	0.1000 (18)
H7A	0.209642	0.883106	0.454527	0.120*
H7B	0.403243	0.766115	0.437452	0.120*
C8	0.2155 (9)	0.4239 (6)	0.43435 (13)	0.0699 (11)
H8A	0.125625	0.325788	0.439510	0.084*
H8B	0.194796	0.453309	0.404928	0.084*
C9	0.4694 (8)	0.3857 (6)	0.44176 (13)	0.0690 (10)
H9A	0.562445	0.483726	0.436549	0.083*
C10	0.5504 (10)	0.2484 (6)	0.41261 (17)	0.0816 (13)
H10A	0.710605	0.222685	0.419194	0.098*
H10B	0.458534	0.151699	0.418309	0.098*
C11	0.5328 (9)	0.2881 (6)	0.36655 (15)	0.0719 (11)
C12	0.3552 (11)	0.2271 (7)	0.34193 (17)	0.0865 (14)
H12A	0.244757	0.158538	0.353907	0.104*
C13	0.3404 (13)	0.2668 (8)	0.29984 (19)	0.1018 (19)
H13A	0.220590	0.224179	0.283566	0.122*
C14	0.4997 (12)	0.3684 (9)	0.28164 (18)	0.1019 (19)
H14A	0.487209	0.395894	0.253249	0.122*
C15	0.6758 (12)	0.4286 (10)	0.3052 (2)	0.106 (2)
H15A	0.785360	0.496659	0.292782	0.128*
C16	0.6946 (9)	0.3899 (8)	0.34768 (18)	0.0894 (14)

H16A	0.816131	0.432318	0.363567	0.107*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.1124 (5)	0.1187 (5)	0.0661 (3)	0.0105 (4)	0.0205 (3)	−0.0022 (3)
N1	0.092 (3)	0.117 (4)	0.064 (2)	−0.005 (3)	−0.018 (2)	0.022 (2)
C1	0.082 (3)	0.059 (2)	0.091 (3)	−0.004 (2)	0.000 (2)	−0.005 (2)
C2	0.081 (3)	0.081 (3)	0.127 (5)	0.015 (3)	0.003 (3)	−0.007 (3)
C3	0.086 (4)	0.092 (4)	0.170 (7)	0.004 (4)	−0.033 (4)	0.008 (5)
C4	0.139 (6)	0.088 (4)	0.112 (5)	−0.024 (4)	−0.037 (5)	0.015 (3)
C5	0.142 (6)	0.087 (3)	0.089 (4)	−0.007 (4)	0.021 (4)	0.008 (3)
C6	0.080 (3)	0.074 (3)	0.093 (3)	0.005 (2)	0.012 (3)	0.010 (2)
C7	0.135 (5)	0.076 (3)	0.089 (3)	−0.006 (3)	−0.007 (4)	−0.011 (3)
C8	0.076 (3)	0.074 (2)	0.060 (2)	−0.006 (2)	−0.0019 (19)	0.0083 (18)
C9	0.075 (3)	0.076 (2)	0.056 (2)	−0.008 (2)	−0.0111 (17)	0.0117 (19)
C10	0.088 (4)	0.073 (2)	0.083 (3)	0.008 (3)	−0.010 (2)	0.006 (2)
C11	0.075 (3)	0.066 (2)	0.075 (2)	0.012 (2)	−0.003 (2)	−0.0074 (19)
C12	0.095 (4)	0.080 (3)	0.085 (3)	−0.005 (3)	−0.008 (3)	−0.013 (2)
C13	0.115 (5)	0.111 (4)	0.079 (3)	−0.003 (4)	−0.017 (3)	−0.026 (3)
C14	0.118 (4)	0.124 (5)	0.064 (3)	0.015 (4)	0.010 (3)	−0.013 (3)
C15	0.104 (4)	0.131 (5)	0.084 (3)	−0.012 (4)	0.026 (3)	−0.007 (3)
C16	0.074 (3)	0.104 (4)	0.091 (3)	−0.001 (3)	0.000 (2)	−0.011 (3)

Geometric parameters (Å, º)

Se1—C8	1.942 (5)	C8—C9	1.515 (7)
Se1—C7	1.979 (7)	C8—H8A	0.9700
N1—C9	1.464 (6)	C8—H8B	0.9700
N1—H1N	0.93 (7)	C9—C10	1.528 (7)
N1—H2N	0.79 (5)	C9—H9A	0.9800
C1—C2	1.361 (8)	C10—C11	1.498 (7)
C1—C6	1.376 (7)	C10—H10A	0.9700
C1—C7	1.504 (8)	C10—H10B	0.9700
C2—C3	1.380 (11)	C11—C12	1.381 (7)
C2—H2A	0.9300	C11—C16	1.387 (8)
C3—C4	1.358 (12)	C12—C13	1.375 (8)
C3—H3A	0.9300	C12—H12A	0.9300
C4—C5	1.361 (11)	C13—C14	1.367 (9)
C4—H4A	0.9300	C13—H13A	0.9300
C5—C6	1.365 (10)	C14—C15	1.354 (10)
C5—H5A	0.9300	C14—H14A	0.9300
C6—H6A	0.9300	C15—C16	1.386 (9)
C7—H7A	0.9700	C15—H15A	0.9300
C7—H7B	0.9700	C16—H16A	0.9300
C8—Se1—C7	97.6 (2)	Se1—C8—H8B	108.6
C9—N1—H1N	103 (4)	H8A—C8—H8B	107.6

C9—N1—H2N	108 (3)	N1—C9—C8	108.8 (4)
H1N—N1—H2N	114 (6)	N1—C9—C10	108.8 (4)
C2—C1—C6	118.8 (5)	C8—C9—C10	110.7 (4)
C2—C1—C7	121.0 (6)	N1—C9—H9A	109.5
C6—C1—C7	120.1 (5)	C8—C9—H9A	109.5
C1—C2—C3	120.5 (6)	C10—C9—H9A	109.5
C1—C2—H2A	119.8	C11—C10—C9	114.1 (4)
C3—C2—H2A	119.8	C11—C10—H10A	108.7
C4—C3—C2	119.9 (6)	C9—C10—H10A	108.7
C4—C3—H3A	120.1	C11—C10—H10B	108.7
C2—C3—H3A	120.1	C9—C10—H10B	108.7
C3—C4—C5	120.2 (7)	H10A—C10—H10B	107.6
C3—C4—H4A	119.9	C12—C11—C16	118.3 (5)
C5—C4—H4A	119.9	C12—C11—C10	121.5 (5)
C4—C5—C6	119.9 (7)	C16—C11—C10	120.3 (5)
C4—C5—H5A	120.1	C13—C12—C11	120.5 (6)
C6—C5—H5A	120.1	C13—C12—H12A	119.7
C5—C6—C1	120.8 (6)	C11—C12—H12A	119.7
C5—C6—H6A	119.6	C14—C13—C12	120.7 (6)
C1—C6—H6A	119.6	C14—C13—H13A	119.6
C1—C7—Se1	112.8 (4)	C12—C13—H13A	119.6
C1—C7—H7A	109.0	C15—C14—C13	119.6 (6)
Se1—C7—H7A	109.0	C15—C14—H14A	120.2
C1—C7—H7B	109.0	C13—C14—H14A	120.2
Se1—C7—H7B	109.0	C14—C15—C16	120.7 (6)
H7A—C7—H7B	107.8	C14—C15—H15A	119.6
C9—C8—Se1	114.6 (3)	C16—C15—H15A	119.6
C9—C8—H8A	108.6	C15—C16—C11	120.2 (5)
Se1—C8—H8A	108.6	C15—C16—H16A	119.9
C9—C8—H8B	108.6	C11—C16—H16A	119.9
C6—C1—C2—C3	−1.4 (8)	N1—C9—C10—C11	−178.8 (4)
C7—C1—C2—C3	177.6 (6)	C8—C9—C10—C11	61.6 (6)
C1—C2—C3—C4	1.2 (10)	C9—C10—C11—C12	−102.5 (6)
C2—C3—C4—C5	−0.5 (11)	C9—C10—C11—C16	76.7 (6)
C3—C4—C5—C6	−0.1 (10)	C16—C11—C12—C13	0.0 (8)
C4—C5—C6—C1	0.0 (9)	C10—C11—C12—C13	179.1 (5)
C2—C1—C6—C5	0.8 (8)	C11—C12—C13—C14	−0.5 (9)
C7—C1—C6—C5	−178.2 (5)	C12—C13—C14—C15	0.9 (10)
C2—C1—C7—Se1	81.1 (6)	C13—C14—C15—C16	−0.8 (11)
C6—C1—C7—Se1	−99.9 (6)	C14—C15—C16—C11	0.2 (10)
Se1—C8—C9—N1	61.1 (5)	C12—C11—C16—C15	0.2 (8)
Se1—C8—C9—C10	−179.4 (3)	C10—C11—C16—C15	−179.0 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···Se1	0.93 (7)	2.69 (7)	3.239 (7)	119 (5)

N1—H2*N*···N1^{i}	0.79 (5)	2.56 (5)	3.319 (5)	161 (4)

Symmetry code: (i) $x+1/2, -y+1/2, -z+1$.