

[(1*S*,2*S*,3*R*,4*R*)-3-Hydroxy-4,7,7-trimethylbicyclo[2.2.1]heptan-2-yl]methyl-[(*E*)-3-(trimethylsilyl)prop-2-enyl]-selenium bromide

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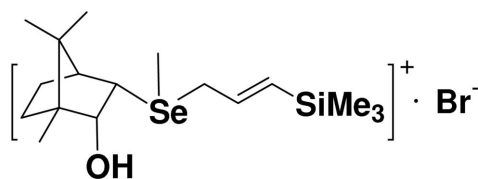
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Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.053; wR factor = 0.103; data-to-parameter ratio = 23.2.

The title compound, a selenium bromide, $\text{C}_{17}\text{H}_{33}\text{OSeSi}^+\cdot\text{Br}^-$, was obtained from the reaction of enantiomerically pure 4,7,7-trimethyl-2-methylselanylbicyclo[2.2.1]heptan-3-ol and (3-bromopropenyl)trimethylsilane in acetone. Due to the chiral bicyclic substituent, the crystal structure is not centrosymmetric and has no symmetry plane, with four chiral C atoms in the cation. The asymmetric unit contains one selenium cation and one bromide anion. $\text{C}-\text{H}\cdots\text{Br}$ and $\text{O}-\text{H}\cdots\text{Br}$ hydrogen bonds link the ions, forming a one-dimensional *R*-helical chain-like supramolecular structure.

Related literature

For related literature, see: Li *et al.* (2005); Goodridge *et al.* (1988); Reich *et al.* (1975); Ye *et al.* (2002).



Experimental

Crystal data

$\text{C}_{17}\text{H}_{33}\text{OSeSi}^+\cdot\text{Br}^-$
 $M_r = 440.39$

Monoclinic, $P2_1$
 $a = 7.555$ (2) Å

$b = 10.023$ (2) Å
 $c = 14.423$ (3) Å
 $\beta = 101.29$ (3)°
 $V = 1071.0$ (4) Å³
 $Z = 2$

Mo $K\alpha$ radiation
 $\mu = 3.67$ mm⁻¹
 $T = 291$ (2) K
 $0.30 \times 0.26 \times 0.24$ mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.35$, $T_{\max} = 0.41$

4460 measured reflections
3374 independent reflections
1732 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.102$
 $S = 1.07$
3374 reflections
170 parameters
1 restraint

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.64$ e Å⁻³
 $\Delta\rho_{\min} = -0.74$ e Å⁻³
Absolute structure: Flack (1983), 1140 Friedel pairs
Flack parameter: 0.01 (2)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1D}\cdots\text{Br1}$	0.87 (8)	2.28 (8)	3.143 (5)	175 (7)
$\text{C5}-\text{H5}\cdots\text{Br1}^{\text{i}}$	0.98	2.88	3.827 (5)	164
$\text{C11}-\text{H11C}\cdots\text{Br1}^{\text{ii}}$	0.96	2.94	3.874 (7)	165
$\text{C12}-\text{H12B}\cdots\text{Br1}^{\text{i}}$	0.97	2.97	3.855 (5)	152

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

Data collection: SMART (Bruker, 2000); cell refinement: SMART; data reduction: SAINT (Bruker, 2000); program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2070).

References

- Bruker (2000). SMART, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Goodridge, R. J., Hambley, T. W., Hayes, R. K. & Ridley, D. D. (1988). *J. Org. Chem.* **53**, 2881–2889.
- Li, X. L., Wang, Y. & Huang, Z. Z. (2005). *Aust. J. Chem.* **58**, 749–752.
- Reich, H. J., Renga, J. M. & Reich, I. J. (1975). *J. Am. Chem. Soc.* **97**, 5434–5447.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Ye, S., Huang, Z. Z., Xia, C. A., Tang, Y. & Dai, L. X. (2002). *J. Am. Chem. Soc.* **124**, 2432–2433.

supplementary materials

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[(1*S*,2*S*,3*R*,4*R*)-3-Hydroxy-4,7,7-trimethylbicyclo[2.2.1]heptan-2-yl]methyl[(*E*)-3-(trimethylsilyl)prop-2-enyl]selenium bromide

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Comment

Recently, an efficient asymmetric synthesis of cyclopropanes *via* camphor-derived sulfonium ylides was reported (Ye *et al.*, 2002). Thus, we expected that camphor-derived selenium ylides could be used in the highly enantioselective synthesis of cyclopropanes, epoxides and aziridines. First, the camphor-derived selenide (1) was prepared from commercially available *D*-camphor according to a literature method (Reich *et al.*, 1975; Goodridge *et al.*, 1988, and Li *et al.*, 2005). Then compound (1) was reacted with (3-bromo-propenyl)-trimethylsilane (3) to give the selenium salt (2). We performed the X-ray crystallographic analysis of (2) in order to elucidate the conformation and configuration.

The structural analysis shows that the selenium ion of the title compound, (2) (Fig. 1), is not centrosymmetric and has no symmetry plane, showing the four chiral C atoms, C4, C5, C6, and C7, with the *R*, *R*, *S*, and *S* configuration preserved from the enantiomerically pure starting compound (1). The asymmetric unit contains one selenium salt cation, and one bromide ion. In the crystal packing, the Br atom plays an important role, acting as a bridge linking neighboring molecules *via* C—H \cdots Br and O—H \cdots Br hydrogen bonds (O1—H1D \cdots Br1, C5—H5 \cdots Br1ⁱⁱ, C11—H11c \cdots Br1ⁱ, and C12—H12B \cdots Br1ⁱⁱ), symmetry code i: $x, -1 + y, z$; ii: $1 - x, -1/2 + y, -z$, forming a one dimensional *R*-helical chains-like structure along [010] axis (Fig. 2).

Experimental

A solution of 4,7,7-trimethyl-2-methylselanyl-bicyclo[2.2.1]heptan-3-ol (1) (2.4 g, 9.7 mmol) and (3-bromo-propenyl)-trimethylsilane (3) (1.9 g, 9.7 mmol) in acetone (5 mL) was stirred at 273 K. The solid was collected and washed with ethyl ether to afford the selenium salt (2) in 91% yield. Single crystals of (2) were obtained by slow evaporation from 10 mL of a methanolic solution containing 50 mg (2).

Refinement

H atoms bonded to O atoms were located in a difference map and refined with distance restraints of O—H = 0.87 (10), and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. Other H atoms were positioned geometrically and refined using a riding model (including free rotation about the ethanol C—C bond), with C—H = 0.96–0.98 Å and with $U_{\text{iso}}(\text{H}) = 1.2(1.5$ for methyl groups) times $U_{\text{eq}}(\text{C})$.

Figures

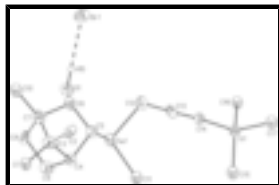


Fig. 1. : View of the title compound, showing the labelling of the non-H atoms and 30% probability ellipsoids. H atoms have been omitted for clarity, except for H1D which is involved in hydrogen bonding.

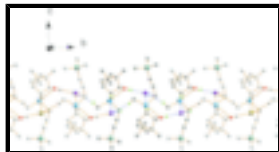


Fig. 2. : A view of the onedimensional *R*-helical chains along the [010] axis. H atoms have been omitted for clarity, except for H1D, H5, H11c, and H12B which are involved in hydrogen bonding.



Fig. 3. : Reaction scheme.

[(1*S*,2*S*,3*R*,4*R*)-3-Hydroxy-4,7,7-trimethylbicyclo[2.2.1]hept-2-yl]methyl[(*E*)-3-(trimethylsilyl)prop-2-enyl]seleniumium bromide

Crystal data

$C_{17}H_{33}OSeSi^+ \cdot Br^-$

$M_r = 440.39$

Monoclinic, $P2(1)$

Hall symbol: P 2yb

$a = 7.555 (2) \text{ \AA}$

$b = 10.023 (2) \text{ \AA}$

$c = 14.423 (3) \text{ \AA}$

$\beta = 101.29 (3)^\circ$

$V = 1071.0 (4) \text{ \AA}^3$

$Z = 2$

$F_{000} = 452$

$D_x = 1.366 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 895 reflections

$\theta = 2.1\text{--}24.5^\circ$

$\mu = 3.67 \text{ mm}^{-1}$

$T = 291 (2) \text{ K}$

Bloc, colourless

$0.30 \times 0.26 \times 0.24 \text{ mm}$

Data collection

Bruker SMART Apex CCD diffractometer

Radiation source: sealed tube

Monochromator: graphite

$T = 291(2) \text{ K}$

phi and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2000)

$T_{\min} = 0.35$, $T_{\max} = 0.41$

4460 measured reflections

3374 independent reflections

1732 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 26.0^\circ$

$\theta_{\min} = 1.4^\circ$

$h = -9 \rightarrow 9$

$k = 0 \rightarrow 12$

$l = 0 \rightarrow 17$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.046P)^2]$
$wR(F^2) = 0.102$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{\max} < 0.001$
3374 reflections	$\Delta\rho_{\max} = 0.64 \text{ e } \text{\AA}^{-3}$
170 parameters	$\Delta\rho_{\min} = -0.74 \text{ e } \text{\AA}^{-3}$
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1140 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.01 (2)

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 $F^2 > \sigma(F^2)$ 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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.32321 (7)	1.05851 (10)	0.09364 (5)	0.0584 (2)
C1	0.6248 (8)	0.4347 (6)	0.3285 (4)	0.0404 (14)
H1A	0.6335	0.3442	0.3079	0.061*
H1B	0.5363	0.4400	0.3679	0.061*
H1C	0.7399	0.4630	0.3637	0.061*
C2	0.7389 (6)	0.5504 (10)	0.2095 (4)	0.0425 (13)
H2A	0.8154	0.6083	0.2529	0.064*
H2B	0.7085	0.5928	0.1488	0.064*
H2C	0.8013	0.4683	0.2036	0.064*
C3	0.5706 (8)	0.5219 (6)	0.2454 (5)	0.0498 (18)
C4	0.4232 (11)	0.4559 (8)	0.1682 (5)	0.0445 (19)
H4	0.4615	0.3724	0.1428	0.053*
C5	0.3867 (6)	0.5695 (8)	0.0960 (4)	0.0361 (12)
H5	0.4822	0.5710	0.0588	0.043*
C6	0.3996 (9)	0.6917 (8)	0.1552 (5)	0.0398 (16)

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H6	0.4963	0.7496	0.1422	0.048*
C7	0.4459 (9)	0.6398 (7)	0.2553 (4)	0.0473 (15)
C8	0.2804 (6)	0.5707 (9)	0.2761 (4)	0.0406 (14)
H8A	0.1744	0.6264	0.2578	0.049*
H8B	0.2955	0.5499	0.3428	0.049*
C9	0.2627 (8)	0.4411 (7)	0.2161 (5)	0.0460 (15)
H9A	0.2728	0.3619	0.2555	0.055*
H9B	0.1499	0.4384	0.1704	0.055*
C10	0.5215 (9)	0.7500 (7)	0.3273 (5)	0.047
H10A	0.6407	0.7741	0.3196	0.071*
H10B	0.5262	0.7175	0.3903	0.071*
H10C	0.4444	0.8269	0.3166	0.071*
C11	0.2014 (9)	0.3828 (7)	-0.0510 (5)	0.043
H11A	0.3020	0.3955	-0.0816	0.064*
H11B	0.0971	0.3576	-0.0970	0.064*
H11C	0.2294	0.3137	-0.0043	0.064*
C12	0.2030 (8)	0.6908 (7)	-0.0809 (4)	0.0415 (15)
H12A	0.1683	0.7780	-0.0614	0.050*
H12B	0.3310	0.6926	-0.0820	0.050*
C13	0.0925 (8)	0.6561 (7)	-0.1810 (4)	0.0430 (15)
H13	-0.0322	0.6663	-0.1918	0.052*
C14	0.1643 (8)	0.6141 (6)	-0.2502 (4)	0.0385 (13)
H14	0.2893	0.6068	-0.2395	0.046*
C15	-0.0572 (9)	0.3993 (7)	-0.3683 (5)	0.047
H15A	-0.1696	0.4027	-0.3468	0.071*
H15B	0.0262	0.3436	-0.3267	0.071*
H15C	-0.0771	0.3631	-0.4311	0.071*
C16	-0.1393 (8)	0.6949 (7)	-0.4057 (5)	0.041
H16A	-0.2022	0.6764	-0.4689	0.061*
H16B	-0.0837	0.7813	-0.4039	0.061*
H16C	-0.2231	0.6937	-0.3636	0.061*
C17	0.1943 (7)	0.5796 (7)	-0.4543 (4)	0.049
H17A	0.2631	0.4987	-0.4522	0.073*
H17B	0.2746	0.6536	-0.4372	0.073*
H17C	0.1259	0.5926	-0.5171	0.073*
O1	0.2297 (6)	0.7626 (5)	0.1376 (3)	0.0473 (11)
H1D	0.248 (10)	0.845 (8)	0.125 (5)	0.057*
Se1	0.15165 (6)	0.54982 (7)	0.01059 (4)	0.04094 (15)
Si1	0.03564 (18)	0.5673 (2)	-0.36882 (11)	0.0395 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0503 (3)	0.0494 (4)	0.0775 (5)	-0.0034 (4)	0.0172 (3)	-0.0074 (5)
C1	0.043 (3)	0.043 (4)	0.040 (3)	0.000 (3)	0.020 (3)	0.000 (3)
C2	0.031 (2)	0.049 (3)	0.043 (3)	-0.012 (4)	-0.0060 (19)	-0.021 (5)
C3	0.038 (3)	0.046 (4)	0.053 (4)	-0.019 (3)	-0.020 (3)	0.003 (3)
C4	0.059 (4)	0.038 (4)	0.034 (4)	-0.005 (3)	0.004 (3)	0.008 (3)

C5	0.035 (2)	0.037 (3)	0.035 (3)	0.019 (3)	0.0062 (18)	0.005 (3)
C6	0.034 (3)	0.048 (4)	0.040 (4)	-0.005 (3)	0.013 (3)	0.003 (3)
C7	0.052 (3)	0.047 (3)	0.037 (4)	0.001 (3)	-0.003 (3)	0.006 (3)
C8	0.042 (2)	0.049 (4)	0.035 (3)	0.016 (3)	0.017 (2)	-0.009 (3)
C9	0.034 (3)	0.046 (4)	0.055 (4)	-0.004 (3)	0.004 (3)	0.005 (3)
C10	0.049	0.049	0.049	0.000	0.021	0.000
C11	0.044	0.044	0.044	0.000	0.018	0.000
C12	0.039 (3)	0.051 (4)	0.036 (3)	0.020 (3)	0.012 (3)	0.009 (3)
C13	0.045 (3)	0.048 (4)	0.033 (3)	0.005 (3)	0.002 (3)	0.014 (3)
C14	0.044 (3)	0.044 (3)	0.029 (3)	-0.004 (2)	0.012 (2)	-0.002 (3)
C15	0.049	0.049	0.049	0.000	0.021	0.000
C16	0.043	0.043	0.043	0.000	0.020	0.000
C17	0.050	0.050	0.050	0.000	0.020	0.000
O1	0.046 (2)	0.049 (3)	0.038 (2)	-0.010 (2)	-0.0126 (19)	0.003 (2)
Se1	0.0358 (2)	0.0516 (3)	0.0339 (3)	0.0028 (4)	0.00292 (19)	0.0086 (4)
Si1	0.0420 (7)	0.0402 (9)	0.0380 (8)	0.0077 (9)	0.0119 (6)	-0.0030 (10)

Geometric parameters (Å, °)

Br1—O1	3.143 (5)	C10—H10B	0.9600
C1—C3	1.475 (9)	C10—H10C	0.9600
C1—H1A	0.9600	C11—Se1	1.965 (7)
C1—H1B	0.9600	C11—H11A	0.9600
C1—H1C	0.9600	C11—H11B	0.9600
C2—C3	1.492 (8)	C11—H11C	0.9600
C2—H2A	0.9600	C12—C13	1.560 (9)
C2—H2B	0.9600	C12—Se1	2.022 (6)
C2—H2C	0.9600	C12—H12A	0.9700
C3—C7	1.535 (9)	C12—H12B	0.9700
C3—C4	1.559 (9)	C13—C14	1.295 (8)
C4—C9	1.515 (10)	C13—H13	0.9300
C4—C5	1.531 (10)	C14—Si1	1.855 (6)
C4—H4	0.9800	C14—H14	0.9300
C5—C6	1.484 (10)	C15—Si1	1.825 (7)
C5—Se1	1.963 (5)	C15—H15A	0.9600
C5—H5	0.9800	C15—H15B	0.9600
C6—O1	1.446 (8)	C15—H15C	0.9600
C6—C7	1.510 (9)	C16—Si1	1.842 (7)
C6—H6	0.9800	C16—H16A	0.9600
C7—C8	1.510 (9)	C16—H16B	0.9600
C7—C10	1.546 (9)	C16—H16C	0.9600
C8—C9	1.552 (10)	C17—Si1	1.884 (5)
C8—H8A	0.9700	C17—H17A	0.9600
C8—H8B	0.9700	C17—H17B	0.9600
C9—H9A	0.9700	C17—H17C	0.9600
C9—H9B	0.9700	O1—H1D	0.87 (8)
C10—H10A	0.9600		
C3—C1—H1A	109.5	C7—C10—H10A	109.5
C3—C1—H1B	109.5	C7—C10—H10B	109.5

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H1A—C1—H1B	109.5	H10A—C10—H10B	109.5
C3—C1—H1C	109.5	C7—C10—H10C	109.5
H1A—C1—H1C	109.5	H10A—C10—H10C	109.5
H1B—C1—H1C	109.5	H10B—C10—H10C	109.5
C3—C2—H2A	109.5	Se1—C11—H11A	109.5
C3—C2—H2B	109.5	Se1—C11—H11B	109.5
H2A—C2—H2B	109.5	H11A—C11—H11B	109.5
C3—C2—H2C	109.5	Se1—C11—H11C	109.5
H2A—C2—H2C	109.5	H11A—C11—H11C	109.5
H2B—C2—H2C	109.5	H11B—C11—H11C	109.5
C1—C3—C2	106.0 (5)	C13—C12—Se1	108.2 (4)
C1—C3—C7	117.3 (6)	C13—C12—H12A	110.1
C2—C3—C7	117.8 (6)	Se1—C12—H12A	110.1
C1—C3—C4	112.0 (5)	C13—C12—H12B	110.1
C2—C3—C4	111.8 (6)	Se1—C12—H12B	110.1
C7—C3—C4	91.6 (5)	H12A—C12—H12B	108.4
C9—C4—C5	109.2 (6)	C14—C13—C12	123.8 (5)
C9—C4—C3	103.9 (6)	C14—C13—H13	118.1
C5—C4—C3	100.3 (5)	C12—C13—H13	118.1
C9—C4—H4	114.0	C13—C14—Si1	124.7 (5)
C5—C4—H4	114.0	C13—C14—H14	117.6
C3—C4—H4	114.0	Si1—C14—H14	117.6
C6—C5—C4	103.8 (5)	Si1—C15—H15A	109.5
C6—C5—Se1	113.2 (4)	Si1—C15—H15B	109.5
C4—C5—Se1	111.9 (5)	H15A—C15—H15B	109.5
C6—C5—H5	109.3	Si1—C15—H15C	109.5
C4—C5—H5	109.3	H15A—C15—H15C	109.5
Se1—C5—H5	109.3	H15B—C15—H15C	109.5
O1—C6—C5	110.4 (5)	Si1—C16—H16A	109.5
O1—C6—C7	111.6 (5)	Si1—C16—H16B	109.5
C5—C6—C7	104.1 (6)	H16A—C16—H16B	109.5
O1—C6—H6	110.2	Si1—C16—H16C	109.5
C5—C6—H6	110.2	H16A—C16—H16C	109.5
C7—C6—H6	110.2	H16B—C16—H16C	109.5
C6—C7—C8	107.5 (5)	Si1—C17—H17A	109.5
C6—C7—C3	102.0 (5)	Si1—C17—H17B	109.5
C8—C7—C3	102.2 (5)	H17A—C17—H17B	109.5
C6—C7—C10	112.5 (6)	Si1—C17—H17C	109.5
C8—C7—C10	114.0 (6)	H17A—C17—H17C	109.5
C3—C7—C10	117.4 (5)	H17B—C17—H17C	109.5
C7—C8—C9	105.0 (5)	C6—O1—Br1	105.8 (4)
C7—C8—H8A	110.8	C6—O1—H1D	109 (5)
C9—C8—H8A	110.8	C5—Se1—C11	98.0 (3)
C7—C8—H8B	110.8	C5—Se1—C12	94.2 (3)
C9—C8—H8B	110.8	C11—Se1—C12	102.9 (3)
H8A—C8—H8B	108.8	C15—Si1—C16	112.8 (3)
C4—C9—C8	100.5 (5)	C15—Si1—C14	111.2 (3)
C4—C9—H9A	111.7	C16—Si1—C14	107.9 (3)
C8—C9—H9A	111.7	C15—Si1—C17	110.9 (3)

C4—C9—H9B	111.7	C16—Si1—C17	106.1 (3)
C8—C9—H9B	111.7	C14—Si1—C17	107.6 (3)
H9A—C9—H9B	109.4		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1D \cdots Br1	0.87 (8)	2.28 (8)	3.143 (5)	175 (7)
C5—H5 \cdots Br1 ⁱ	0.98	2.88	3.827 (5)	164
C11—H11C \cdots Br1 ⁱⁱ	0.96	2.94	3.874 (7)	165
C12—H12B \cdots Br1 ⁱ	0.97	2.97	3.855 (5)	152

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

Fig. 1

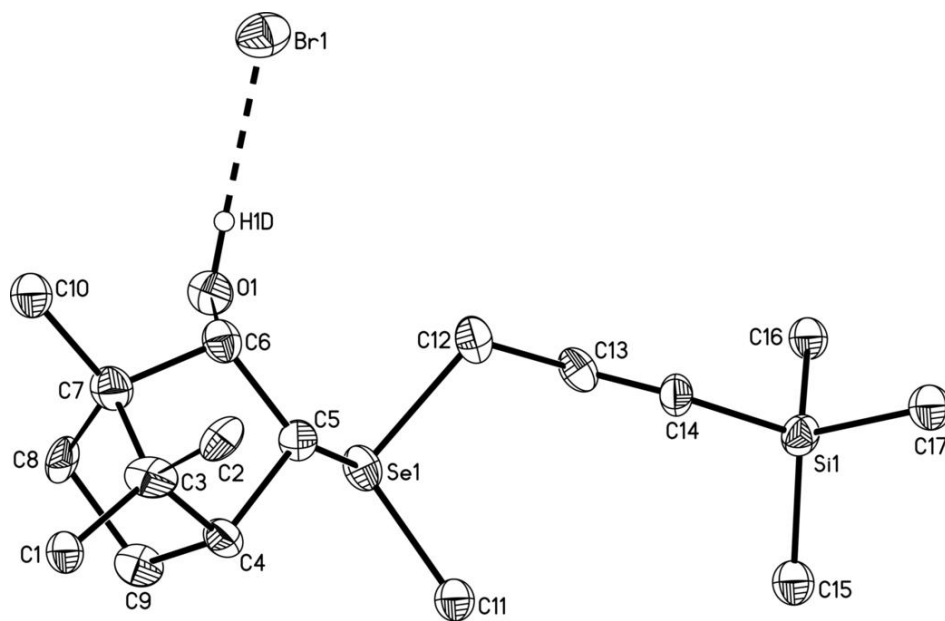


Fig. 2

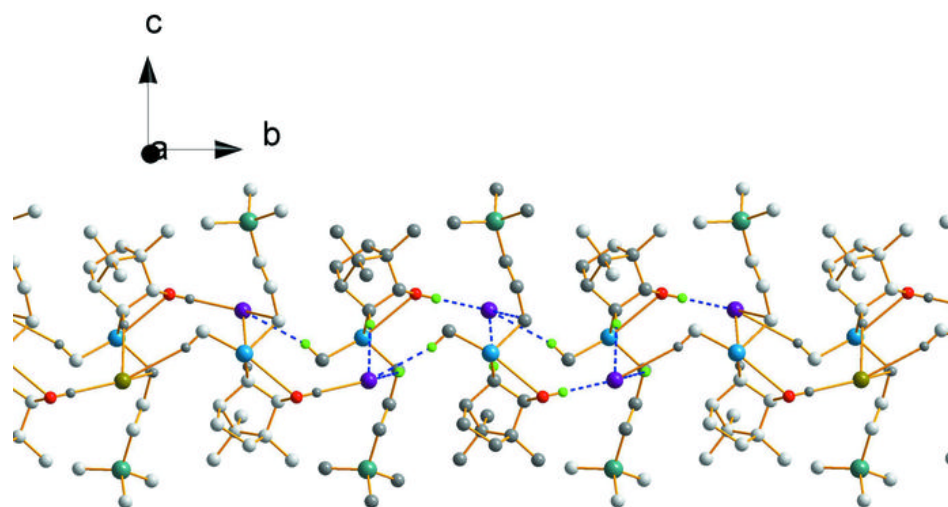


Fig. 3

