

Bis[bis[2-(dimethylaminomethyl)phenyl]-hydroxytelluronium] hexafluorosilicate chloroform tetrasolvate

Thomas M. Klapötke,* Burkhard Krumm and Matthias Scherr

Department of Chemistry and Biochemistry, Ludwig-Maximilian University, Butenandtstrasse 5–13, D-81377 Munich, Germany

Correspondence e-mail: tmk@cup.uni-muenchen.de

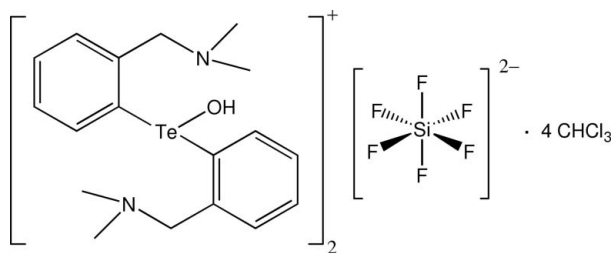
Received 25 September 2007; accepted 26 September 2007

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.022; wR factor = 0.053; data-to-parameter ratio = 16.8.

In the structure of the title compound $2\text{C}_{18}\text{H}_{25}\text{N}_2\text{OTe}^{+}\cdot\text{SiF}_6^{2-}\cdot 4\text{CHCl}_3$, the bis[2-(dimethylaminomethyl)phenyl]-hydroxytelluronium cations and $[\text{SiF}_6]^{2-}$ anions are linked via an intermolecular $\text{O}-\text{H}\cdots\text{F}$ hydrogen bond and a secondary intermolecular interaction between Te and F [2.890 (2) Å].

Related literature

For related literature, see: Beckmann *et al.* (2005); Bondi (1964); Hammerl *et al.* (2007).



Experimental

Crystal data

$2\text{C}_{18}\text{H}_{25}\text{N}_2\text{OTe}^{+}\cdot\text{F}_6\text{Si}^{2-}\cdot 4\text{CHCl}_3$
 $M_r = 1445.56$
 Monoclinic, $P2_1/c$
 $a = 9.3260$ (2) Å

$b = 26.7485$ (5) Å
 $c = 12.1579$ (3) Å
 $\beta = 112.310$ (3)°
 $V = 2805.84$ (12) Å³

$Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.69$ mm⁻¹

$T = 100$ (2) K
 $0.27 \times 0.17 \times 0.16$ mm

Data collection

Oxford Xcalibur3 CCD area-detector diffractometer
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
 $T_{\min} = 0.682$, $T_{\max} = 0.760$

12419 measured reflections
 5303 independent reflections
 4543 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.053$
 $S = 1.03$
 5303 reflections
 316 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.70$ e Å⁻³
 $\Delta\rho_{\min} = -0.47$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{F1}$	0.84 (2)	1.86 (2)	2.696 (2)	177 (3)

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1996); software used to prepare material for publication: *SHELXL97*.

The University of Munich, the Fonds der Chemischen Industrie and the Deutsche Forschungsgemeinschaft (KL 636/10-1) are gratefully acknowledged for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2520).

References

- Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
- Beckmann, J., Dakternieks, D., Duthie, A., Lewcenko, N. A., Mitchell, C. & Schürmann, M. (2005). *Z. Anorg. Allg. Chem.* **631**, 1586–1862.
- Bondi, A. (1964). *J. Phys. Chem.* **68**, 441–451.
- Brandenburg, K. (1996). *DIAMOND*. University of Bonn, Germany.
- Hammerl, A., Klapötke, T. M., Krumm, B. & Scherr, M. (2007). *Z. Anorg. Allg. Chem.* **633**, 1618–1626.
- Oxford Diffraction (2006). *CrysAlis CCD* and *CrysAlis RED*. Versions 1.171. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E63, o4189 [doi:10.1107/S1600536807047253]

Bis{bis[2-(dimethylaminomethyl)phenyl]hydroxytelluronium} hexafluorosilicate chloroform tetrasolvate

T. M. Klapötke, B. Krumm and M. Scherr

Comment

As part of our recent studies regarding tellurium(II) and tellurium(IV) compounds with the intramolecular donor stabilizing substituent 2-Me₂NCH₂C₆H₄ (Hammerl *et al.*, 2007) we obtained the title compound as a decomposition product.

In the title compound two intramolecular interactions between the aminomethyl nitrogen atom and the tellurium atom create two five-membered heterocycles with a 4-coordinated amine moiety (Te1...N1 2.719 (3) and Te1...N2 2.557 (2) Å). The Te1–O1 distance is with 1.9612 (17) Å slightly elongated compared to the calculated bond distance in [Ph₂TeOH]⁺ (1.937 Å, Beckmann *et al.*, 2005). The present hydrogen bridge O1–H1...F1 links the cation with the anion and exhibits a donor acceptor distance of 2.696 (2) Å. The tellurium atom is further coordinated by an intermolecular tellurium–fluorine interaction (Te1–Fⁱ) 2.890 (2) Å which is significantly shorter than the sum of the tellurium–fluorine van der Waals radii (3.53 Å, Bondi 1964).

Experimental

The tellurium(IV) difluoride (2-Me₂NCH₂C₆H₄)₂TeF₂ was prepared according to literature (Hammerl *et al.*, 2007). A solution in chloroform stored for a period of 3 months in a glass vessel at 4°C results in the formation of colorless crystals of the title compound suitable for X-ray diffraction studies. The presence of Si in the structure results from the slow reaction of the tellurium(IV) difluoride with glass.

Refinement

H atoms were refined with fixed individual displacement parameters [$U(H) = 1.2U_{eq}(C)$ or $U(H) = 1.5U_{eq}(C_{methyl})$] using a riding model with C–H ranging from 0.95 Å, to 1.00 Å. The H atom bonded to O was freely refined.

Figures

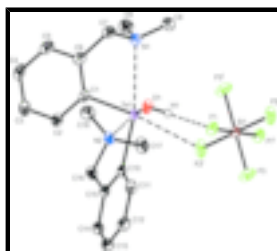


Fig. 1. Molecular structure of [(2-Me₂NCH₂C₆H₄)₂TeOH]₂SiF₆ with displacement ellipsoids drawn at the 50% probability level, solvent molecules not shown. Symmetry code: (i) 2 - x, -y, 2 - z.

supplementary materials

Bis[bis[2-(dimethylaminomethyl)phenyl]hydroxytelluronium] hexafluorosilicate chloroform tetrasolvate

Crystal data

$2C_{18}H_{25}N_2O_2Te^+ \cdot F_6Si^{2-} \cdot 4CHCl_3$	$F_{000} = 1428$
$M_r = 1445.56$	$D_x = 1.711 (1) \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 9.3260 (2) \text{ \AA}$	Cell parameters from 10976 reflections
$b = 26.7485 (5) \text{ \AA}$	$\theta = 3.8\text{--}30.0^\circ$
$c = 12.1579 (3) \text{ \AA}$	$\mu = 1.69 \text{ mm}^{-1}$
$\beta = 112.310 (3)^\circ$	$T = 100 (2) \text{ K}$
$V = 2805.84 (12) \text{ \AA}^3$	Block, colourless
$Z = 2$	$0.27 \times 0.17 \times 0.16 \text{ mm}$

Data collection

Oxford Xcalibur3 CCD area-detector diffractometer	5303 independent reflections
Radiation source: fine-focus sealed tube	4543 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.020$
Detector resolution: $15.9809 \text{ pixels mm}^{-1}$	$\theta_{\text{max}} = 26.0^\circ$
$T = 100(2) \text{ K}$	$\theta_{\text{min}} = 3.8^\circ$
ω scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2006)	$k = -32 \rightarrow 32$
$T_{\text{min}} = 0.682$, $T_{\text{max}} = 0.760$	$l = -15 \rightarrow 14$
12419 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.022$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.0248P)^2 + 1.7973P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
5303 reflections	$(\Delta/\sigma)_{\text{max}} = 0.002$
316 parameters	$\Delta\rho_{\text{max}} = 0.70 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.47 \text{ e \AA}^{-3}$
	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. Details of H atom refinement: H atoms were placed in idealized positions and allowed to ride on their respective parent atoms, with C–H = 0.95 (C_{arom}H), 1.00 (CH), 0.99 (CH₂), 0.98 Å (CH₃) and with $U_{\text{iso}}(\text{H}) = kU_{\text{eq}}(\text{carrier atom})$, where $k = 1.2$ for CH₂ and CH, and 1.5 for CH₃. Atom H1 was located in a difference Fourier map and the position refined with the restraint O–H = 0.84 Å. The highest peak and deepest hole in the final difference map were located 0.82 and 0.77 Å, respectively, from atom Cl6.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Te1	0.657332 (16)	0.106265 (5)	0.882461 (12)	0.01500 (5)
N2	0.3736 (2)	0.08058 (7)	0.82241 (16)	0.0177 (4)
N1	0.7151 (2)	0.13877 (7)	0.69141 (17)	0.0211 (4)
C14	0.4448 (3)	0.08912 (9)	1.1451 (2)	0.0234 (5)
H14	0.3442	0.0823	1.1437	0.028*
O1	0.86846 (18)	0.13175 (6)	0.96468 (14)	0.0206 (3)
C16	0.3275 (3)	0.09072 (9)	0.9225 (2)	0.0210 (5)
H16A	0.2564	0.0641	0.9270	0.025*
H16B	0.2706	0.1229	0.9088	0.025*
C13	0.5689 (3)	0.09495 (9)	1.2530 (2)	0.0256 (5)
H13	0.5528	0.0921	1.3251	0.031*
C1	0.5838 (2)	0.18220 (8)	0.84948 (19)	0.0161 (4)
C9	0.5761 (3)	0.12922 (10)	0.5851 (2)	0.0281 (6)
H9A	0.5643	0.0931	0.5704	0.042*
H9B	0.5858	0.1459	0.5168	0.042*
H9C	0.4847	0.1422	0.5967	0.042*
C6	0.6282 (3)	0.21139 (9)	0.7725 (2)	0.0199 (5)
C18	0.2607 (3)	0.10074 (10)	0.7101 (2)	0.0278 (6)
H18A	0.2953	0.0933	0.6455	0.042*
H18B	0.2526	0.1370	0.7171	0.042*
H18C	0.1588	0.0854	0.6927	0.042*
C17	0.3917 (3)	0.02619 (9)	0.8115 (2)	0.0274 (6)
H17A	0.4229	0.0196	0.7448	0.041*
H17B	0.2927	0.0094	0.7974	0.041*
H17C	0.4716	0.0134	0.8851	0.041*
C7	0.7367 (3)	0.19189 (9)	0.7170 (2)	0.0221 (5)
H7A	0.7180	0.2103	0.6423	0.026*
H7B	0.8455	0.1981	0.7718	0.026*
C10	0.6168 (3)	0.10249 (8)	1.0427 (2)	0.0166 (4)
C4	0.4903 (3)	0.28133 (9)	0.8102 (2)	0.0283 (6)
H4	0.4561	0.3150	0.7949	0.034*
C5	0.5788 (3)	0.26103 (9)	0.7539 (2)	0.0267 (5)
H5	0.6070	0.2812	0.7012	0.032*

supplementary materials

C12	0.7166 (3)	0.10490 (9)	1.2563 (2)	0.0255 (5)
H12	0.8009	0.1095	1.3305	0.031*
C8	0.8526 (3)	0.11594 (10)	0.6818 (3)	0.0317 (6)
H8A	0.8338	0.0802	0.6648	0.048*
H8B	0.9423	0.1203	0.7569	0.048*
H8C	0.8736	0.1320	0.6174	0.048*
C11	0.7411 (3)	0.10819 (9)	1.1516 (2)	0.0222 (5)
H11	0.8426	0.1143	1.1540	0.027*
C15	0.4664 (3)	0.09319 (8)	1.0388 (2)	0.0179 (5)
C2	0.4969 (3)	0.20344 (8)	0.9081 (2)	0.0201 (5)
H2	0.4690	0.1838	0.9617	0.024*
C3	0.4509 (3)	0.25304 (9)	0.8888 (2)	0.0253 (5)
H3	0.3924	0.2675	0.9295	0.030*
Si1	1.0000	0.0000	1.0000	0.01539 (18)
F1	1.07064 (15)	0.05684 (5)	1.06107 (11)	0.0210 (3)
F2	1.17733 (16)	-0.01661 (5)	1.00741 (14)	0.0320 (3)
F3	1.04137 (18)	-0.02414 (5)	1.13490 (12)	0.0310 (3)
Cl4	0.97905 (14)	0.29009 (3)	0.96386 (8)	0.0668 (3)
Cl6	1.18389 (9)	0.20509 (4)	1.02213 (8)	0.0558 (2)
C20	1.0230 (3)	0.23273 (10)	1.0382 (2)	0.0285 (6)
H20	0.9316	0.2100	1.0020	0.034*
Cl2	0.18542 (8)	0.11551 (2)	0.34050 (7)	0.03729 (16)
Cl3	0.34958 (8)	0.02133 (3)	0.38681 (7)	0.03718 (16)
Cl5	1.05725 (9)	0.24076 (3)	1.18901 (6)	0.0486 (2)
Cl1	0.05482 (9)	0.02905 (3)	0.40971 (7)	0.04611 (19)
C19	0.1657 (3)	0.05000 (9)	0.3308 (2)	0.0237 (5)
H19	0.1112	0.0405	0.2453	0.028*
H1	0.930 (3)	0.1078 (7)	0.992 (2)	0.031 (8)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Te1	0.01481 (8)	0.01247 (8)	0.01868 (8)	0.00000 (6)	0.00752 (6)	0.00070 (6)
N2	0.0176 (10)	0.0158 (10)	0.0204 (9)	-0.0004 (8)	0.0082 (8)	-0.0016 (8)
N1	0.0251 (11)	0.0199 (10)	0.0217 (10)	0.0011 (8)	0.0129 (9)	0.0021 (8)
C14	0.0322 (14)	0.0148 (11)	0.0296 (13)	0.0004 (10)	0.0191 (11)	0.0003 (10)
O1	0.0148 (8)	0.0165 (8)	0.0285 (9)	0.0005 (7)	0.0062 (7)	0.0028 (7)
C16	0.0189 (12)	0.0194 (12)	0.0273 (12)	-0.0010 (9)	0.0119 (10)	-0.0011 (10)
C13	0.0403 (15)	0.0192 (12)	0.0217 (12)	0.0033 (11)	0.0168 (11)	-0.0011 (10)
C1	0.0150 (11)	0.0133 (11)	0.0171 (11)	0.0000 (8)	0.0030 (9)	0.0010 (9)
C9	0.0355 (15)	0.0259 (13)	0.0232 (12)	-0.0027 (11)	0.0117 (11)	-0.0026 (11)
C6	0.0198 (12)	0.0191 (11)	0.0175 (11)	-0.0037 (9)	0.0036 (9)	0.0008 (9)
C18	0.0191 (12)	0.0390 (15)	0.0220 (12)	-0.0011 (11)	0.0044 (10)	0.0006 (11)
C17	0.0305 (14)	0.0168 (12)	0.0392 (15)	-0.0064 (10)	0.0182 (12)	-0.0068 (11)
C7	0.0261 (13)	0.0193 (12)	0.0223 (12)	-0.0038 (10)	0.0110 (10)	0.0028 (10)
C10	0.0216 (11)	0.0107 (10)	0.0199 (11)	0.0028 (9)	0.0105 (9)	0.0019 (9)
C4	0.0368 (15)	0.0127 (11)	0.0327 (14)	0.0026 (10)	0.0105 (12)	0.0019 (10)
C5	0.0353 (14)	0.0175 (12)	0.0255 (12)	-0.0035 (11)	0.0098 (11)	0.0053 (10)

C12	0.0358 (14)	0.0199 (12)	0.0179 (11)	0.0015 (11)	0.0073 (11)	-0.0021 (10)
C8	0.0366 (15)	0.0326 (15)	0.0355 (15)	0.0094 (12)	0.0246 (13)	0.0085 (12)
C11	0.0223 (12)	0.0179 (12)	0.0251 (12)	0.0018 (10)	0.0078 (10)	-0.0002 (10)
C15	0.0223 (12)	0.0099 (10)	0.0230 (12)	0.0005 (9)	0.0106 (10)	0.0003 (9)
C2	0.0199 (12)	0.0167 (11)	0.0236 (12)	-0.0004 (9)	0.0082 (10)	0.0021 (9)
C3	0.0291 (14)	0.0165 (12)	0.0303 (13)	0.0017 (10)	0.0115 (11)	-0.0026 (10)
Si1	0.0146 (4)	0.0148 (4)	0.0151 (4)	0.0008 (3)	0.0038 (3)	0.0011 (3)
F1	0.0208 (7)	0.0178 (7)	0.0202 (7)	0.0000 (5)	0.0032 (6)	0.0005 (5)
F2	0.0208 (8)	0.0208 (7)	0.0573 (10)	0.0026 (6)	0.0183 (7)	0.0015 (7)
F3	0.0509 (10)	0.0212 (7)	0.0166 (7)	-0.0042 (7)	0.0084 (7)	0.0035 (6)
Cl4	0.1229 (9)	0.0308 (4)	0.0442 (5)	0.0042 (5)	0.0295 (5)	0.0048 (3)
Cl6	0.0359 (4)	0.0773 (6)	0.0648 (5)	-0.0022 (4)	0.0311 (4)	-0.0307 (5)
C20	0.0310 (14)	0.0265 (13)	0.0319 (14)	-0.0031 (11)	0.0165 (12)	-0.0046 (11)
Cl2	0.0358 (4)	0.0240 (3)	0.0439 (4)	-0.0009 (3)	0.0063 (3)	-0.0025 (3)
Cl3	0.0264 (3)	0.0305 (3)	0.0503 (4)	0.0026 (3)	0.0101 (3)	0.0028 (3)
Cl5	0.0502 (5)	0.0688 (5)	0.0305 (4)	0.0299 (4)	0.0197 (3)	0.0049 (4)
Cl1	0.0460 (4)	0.0547 (5)	0.0493 (4)	-0.0008 (4)	0.0312 (4)	0.0102 (4)
C19	0.0254 (13)	0.0230 (13)	0.0216 (12)	-0.0005 (10)	0.0077 (10)	0.0011 (10)

Geometric parameters (Å, °)

Te1—O1	1.9612 (17)	C17—H17C	0.9800
Te1—C10	2.123 (2)	C7—H7A	0.9900
Te1—C1	2.132 (2)	C7—H7B	0.9900
Te1—N2	2.557 (2)	C10—C11	1.398 (3)
Te1—N1	2.719 (3)	C10—C15	1.407 (3)
N2—C16	1.462 (3)	C4—C5	1.373 (4)
N2—C18	1.474 (3)	C4—C3	1.378 (3)
N2—C17	1.477 (3)	C4—H4	0.9500
N1—C7	1.452 (3)	C5—H5	0.9500
N1—C9	1.464 (3)	C12—C11	1.379 (3)
N1—C8	1.465 (3)	C12—H12	0.9500
C14—C13	1.390 (3)	C8—H8A	0.9800
C14—C15	1.386 (3)	C8—H8B	0.9800
C14—H14	0.9500	C8—H8C	0.9800
O1—H1	0.84 (2)	C11—H11	0.9500
C16—C15	1.514 (3)	C2—C3	1.386 (3)
C16—H16A	0.9900	C2—H2	0.9500
C16—H16B	0.9900	C3—H3	0.9500
C13—C12	1.388 (4)	Si1—F3 ⁱ	1.6659 (14)
C13—H13	0.9500	Si1—F3	1.6659 (14)
C1—C2	1.388 (3)	Si1—F2	1.6808 (13)
C1—C6	1.397 (3)	Si1—F2 ⁱ	1.6808 (13)
C9—H9A	0.9800	Si1—F1 ⁱ	1.7091 (13)
C9—H9B	0.9800	Si1—F1	1.7091 (13)
C9—H9C	0.9800	Cl4—C20	1.748 (3)
C6—C5	1.395 (3)	Cl6—C20	1.750 (3)
C6—C7	1.511 (3)	C20—Cl5	1.751 (2)

supplementary materials

C18—H18A	0.9800	C20—H20	1.0000
C18—H18B	0.9800	C12—C19	1.761 (2)
C18—H18C	0.9800	C13—C19	1.762 (3)
C17—H17A	0.9800	C11—C19	1.748 (3)
C17—H17B	0.9800	C19—H19	1.0000
O1—Te1—C10	92.46 (9)	C6—C7—H7A	109.2
O1—Te1—C1	87.35 (7)	N1—C7—H7B	109.2
C10—Te1—C1	93.44 (8)	C6—C7—H7B	109.2
O1—Te1—N2	165.62 (6)	H7A—C7—H7B	107.9
C10—Te1—N2	73.97 (8)	C11—C10—C15	120.6 (2)
C1—Te1—N2	88.75 (7)	C11—C10—Te1	119.44 (17)
O1—Te1—N2	165.62 (6)	C15—C10—Te1	119.99 (17)
C10—Te1—N2	73.97 (8)	C5—C4—C3	120.0 (2)
C1—Te1—N2	88.75 (7)	C5—C4—H4	119.9
O1—Te1—N1	80.68 (6)	C3—C4—H4	119.9
C10—Te1—N1	163.99 (7)	C4—C5—C6	121.3 (2)
C1—Te1—N1	71.86 (7)	C4—C5—H5	119.3
N1—Te1—N2	111.17 (6)	C6—C5—H5	119.3
C16—N2—C18	111.85 (18)	C11—C12—C13	119.7 (2)
C16—N2—C17	109.71 (18)	C11—C12—H12	120.0
C18—N2—C17	110.1 (2)	C13—C12—H12	120.0
C16—N2—Te1	108.18 (14)	N1—C8—H8A	109.5
C18—N2—Te1	117.65 (15)	N1—C8—H8B	109.5
C17—N2—Te1	98.58 (14)	H8A—C8—H8B	109.5
C7—N1—C9	111.36 (19)	N1—C8—H8C	109.5
C7—N1—C8	111.8 (2)	H8A—C8—H8C	109.5
C9—N1—C8	111.2 (2)	H8B—C8—H8C	109.5
C13—C14—C15	120.5 (2)	C12—C11—C10	119.9 (2)
C13—C14—H14	119.7	C12—C11—H11	120.0
C15—C14—H14	119.7	C10—C11—H11	120.0
Te1—O1—H1	110 (2)	C14—C15—C10	118.6 (2)
N2—C16—C15	111.64 (18)	C14—C15—C16	119.5 (2)
N2—C16—H16A	109.3	C10—C15—C16	121.9 (2)
C15—C16—H16A	109.3	C3—C2—C1	120.4 (2)
N2—C16—H16B	109.3	C3—C2—H2	119.8
C15—C16—H16B	109.3	C1—C2—H2	119.8
H16A—C16—H16B	108.0	C4—C3—C2	119.7 (2)
C14—C13—C12	120.7 (2)	C4—C3—H3	120.1
C14—C13—H13	119.9	C2—C3—H3	120.1
C12—C13—H13	119.9	F3 ⁱ —Si1—F3	180.0
C2—C1—C6	119.9 (2)	F3 ⁱ —Si1—F2	90.61 (8)
C2—C1—Te1	120.04 (16)	F3—Si1—F2	89.39 (8)
C6—C1—Te1	120.04 (16)	F3 ⁱ —Si1—F2 ⁱ	89.39 (8)
N1—C9—H9A	109.5	F3—Si1—F2 ⁱ	90.61 (8)
N1—C9—H9B	109.5	F2—Si1—F2 ⁱ	180.0
H9A—C9—H9B	109.5	F3 ⁱ —Si1—F1 ⁱ	90.58 (6)
N1—C9—H9C	109.5	F3—Si1—F1 ⁱ	89.42 (6)

H9A—C9—H9C	109.5	F2—Si1—F1 ⁱ	89.85 (7)
H9B—C9—H9C	109.5	F2 ⁱ —Si1—F1 ⁱ	90.16 (7)
C5—C6—C1	118.4 (2)	F3 ⁱ —Si1—F1	89.42 (6)
C5—C6—C7	119.5 (2)	F3—Si1—F1	90.58 (6)
C1—C6—C7	122.0 (2)	F2—Si1—F1	90.16 (7)
N2—C18—H18A	109.5	F2 ⁱ —Si1—F1	89.85 (7)
N2—C18—H18B	109.5	F1 ⁱ —Si1—F1	180.00 (4)
H18A—C18—H18B	109.5	C14—C20—C16	110.85 (16)
N2—C18—H18C	109.5	C14—C20—C15	110.32 (14)
H18A—C18—H18C	109.5	C16—C20—C15	110.22 (14)
H18B—C18—H18C	109.5	C14—C20—H20	108.4
N2—C17—H17A	109.5	C16—C20—H20	108.4
N2—C17—H17B	109.5	C15—C20—H20	108.4
H17A—C17—H17B	109.5	C11—C19—C13	109.93 (13)
N2—C17—H17C	109.5	C11—C19—C12	110.45 (13)
H17A—C17—H17C	109.5	C13—C19—C12	110.30 (13)
H17B—C17—H17C	109.5	C11—C19—H19	108.7
N1—C7—C6	111.86 (19)	C13—C19—H19	108.7
N1—C7—H7A	109.2	C12—C19—H19	108.7
O1—Te1—N2—C16	-4.3 (3)	C1—C6—C7—N1	34.1 (3)
C10—Te1—N2—C16	15.43 (14)	O1—Te1—C10—C11	-11.54 (18)
C1—Te1—N2—C16	-78.50 (14)	C1—Te1—C10—C11	-98.90 (18)
O1—Te1—N2—C18	123.6 (3)	N2—Te1—C10—C11	173.30 (19)
C10—Te1—N2—C18	143.28 (17)	O1—Te1—C10—C15	169.89 (17)
C1—Te1—N2—C18	49.36 (17)	C1—Te1—C10—C15	82.53 (18)
O1—Te1—N2—C17	-118.5 (3)	N2—Te1—C10—C15	-5.27 (16)
C10—Te1—N2—C17	-98.76 (15)	C3—C4—C5—C6	1.3 (4)
C1—Te1—N2—C17	167.31 (15)	C1—C6—C5—C4	0.7 (4)
C18—N2—C16—C15	-153.0 (2)	C7—C6—C5—C4	-174.8 (2)
C17—N2—C16—C15	84.5 (2)	C14—C13—C12—C11	-1.1 (4)
Te1—N2—C16—C15	-22.1 (2)	C13—C12—C11—C10	1.3 (3)
C15—C14—C13—C12	-0.1 (4)	C15—C10—C11—C12	-0.2 (3)
O1—Te1—C1—C2	-109.56 (18)	Te1—C10—C11—C12	-178.82 (17)
C10—Te1—C1—C2	-17.04 (18)	C13—C14—C15—C10	1.1 (3)
N2—Te1—C1—C2	56.51 (18)	C13—C14—C15—C16	-175.2 (2)
O1—Te1—C1—C6	67.85 (18)	C11—C10—C15—C14	-0.9 (3)
C10—Te1—C1—C6	160.37 (18)	Te1—C10—C15—C14	177.65 (16)
N2—Te1—C1—C6	-126.08 (18)	C11—C10—C15—C16	175.3 (2)
C2—C1—C6—C5	-2.1 (3)	Te1—C10—C15—C16	-6.1 (3)
Te1—C1—C6—C5	-179.50 (17)	N2—C16—C15—C14	-162.94 (19)
C2—C1—C6—C7	173.3 (2)	N2—C16—C15—C10	20.9 (3)
Te1—C1—C6—C7	-4.1 (3)	C6—C1—C2—C3	1.5 (3)
C9—N1—C7—C6	76.6 (2)	Te1—C1—C2—C3	178.88 (18)
C8—N1—C7—C6	-158.1 (2)	C5—C4—C3—C2	-2.0 (4)
C5—C6—C7—N1	-150.6 (2)	C1—C2—C3—C4	0.6 (4)

Symmetry codes: (i) $-x+2, -y, -z+2$.

supplementary materials

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1—H1···F1	0.84 (2)	1.86 (2)	2.696 (2)	177 (3)

Fig. 1

