organic compounds

Bis(1-naphthyl) telluride

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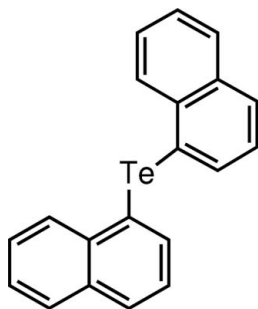Correspondence e-mail: akschauhan2003@yahoo.co.in

Yellow crystals of the title compound, $C_{20}H_{14}Te$, were obtained serendipitously in an attempt to recrystallize the reduction product of $(1\text{-}C_{10}H_7)[(CH(Me)COC_6H_5)]TeCl_2$ from dichloromethane. The molecule exhibits an angular geometry with almost equal Te—C_{aryl} bonds and a C—Te—C angle close to values observed for other diaryl tellurides. One of the aromatic ring systems lies in the C—Te—C plane and the other is oriented at 76.81 (6)°, giving an almost T-shaped conformation that is compatible with the steric demand of 1-naphthyl ligands.

Related literature

For related literature, see: Lyons *et al.* (1908); Arnauld *et al.* (1999); Akiba *et al.* (1984); Farran *et al.* (1997); Engman *et al.* (2002); Klapötke *et al.* (2005); Voelker *et al.* (1999); Wieber *et al.* (1995); Allen *et al.* (1987, 2002); Schulz Lang *et al.* (2002).

Experimental

Crystal data

$C_{20}H_{14}Te$	V = 3034.8 (2) Å^3
M_r = 381.91	Z = 8
Orthorhombic, $Pbca$	Mo $K\alpha$ radiation
a = 14.0662 (6) Å	μ = 1.95 mm^{-1}
b = 8.7390 (4) Å	T = 130 (2) K
c = 24.6881 (11) Å	0.45 × 0.40 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer	11725 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	3477 independent reflections
T_{min} = 0.460, T_{max} = 0.676	3158 reflections with $I > 2\sigma(I)$
	R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028	190 parameters
$wR(F^2)$ = 0.073	H-atom parameters constrained
S = 1.06	$\Delta\rho_{max}$ = 1.05 e Å^{-3}
3477 reflections	$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—Te	2.119 (2)	C11—Te	2.119 (2)
C1—Te—C11	96.32 (9)		
C2—C1—Te—C11	105.2 (2)	C12—C11—Te—C1	−2.4 (2)
C10—C1—Te—C11	−77.9 (2)	C20—C11—Te—C1	179.90 (17)

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenberg & Putz, 2006); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2027).

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supplementary materials

Bis(1-naphthyl) telluride

A. K. S. Chauhan, Anamika, R. C. Srivastava and A. Duthie

Comment

The molecule of the title compound, (**I**) (Fig.1), adopts angular geometry similar to other symmetrical diaryltellurides, $(4-XC_6H_5)_2Te$, X = OMe (Farran *et al.*, 1997); X = OH, NH_2, NMe_2 (Engman *et al.*, 2002). Both Te—C_{aryl} bonds are 2.119 (2) Å and inclined at 96.32 (9)^0. These bond parameters are quite close to the reported average values of 2.116 (20) Å (Allen, *et al.*, 1987) and 96 (3)^0 (Allen *et al.*, 1993) which indicate little steric influence of 1-naphthyl ligands on the molecular geometry of (**I**). With sterically more demanding aryl ligands enlarged values for these bond parameters have been reported in the case of mesityl [2.140 (3) Å each, 101.0 (1)^0 (Klapötke *et al.*, 2005)], nonafluoromesityl [2.151 (5) Å each, 107.4 (2)^0 (Voelker *et al.*, 1999)] and supermesityl [2.156 (5) Å, 2.157 (5) Å, 107.3 (2)^0 (Wieber *et al.*, 1995)] analogues. However, the almost T-shaped conformation adopted by the molecule with an interplanar angle of 79.87 (4)^0 between the planar [to within 0.005 (5) and 0.014 (7) Å] naphthalene rings may be attributed to steric repulsion between 1-naphthyl ligands.

The centroids of the four aromatic rings, defined as *Cg*1 (C1—C4, C9—C10), *Cg*2 (C5—C10), *Cg*3 (C11—C14, C19—C20) and *Cg*4 (C15—C20) are involved in the crystal packing of (**I**). Centrosymmetric pairs of molecules joined by reciprocal π(*Cg*1)···π(*Cg*2) interactions of 3.875 (1) Å (symmetry code: $1 - x$, $- y$, $1 - z$) are further connected *via* a Te···π(*Cg*2) = 3.9567 (2) Å (symmetry code: $1 - x$, $- y$, $1 - z$) contact and four C—H···π(ring centroid) interactions [C4—H4···π(*Cg*2) = 2.748 Å (symmetry code: $1/2 - x$, $1/2 + y$, z), C7—H7···π(*Cg*3) = 2.772 Å (symmetry code: $1 - x$, $1 - y$, $1 - z$), C15—H15···π(*Cg*3) = 2.724 Å (symmetry code: $1 - x$, $-1/2 + y$, $1/2 - z$)) and C6—H6···π(*Cg*4) = 2.852 Å (symmetry code: $1 - x$, $1 - y$, $1 - z$)] to form a three-dimensional network.

Bis(1-naphthyl)telluride, prepared earlier by the transfer of aryl ligands from $(1-C_{10}H_7)_2Hg$ (Lyons *et al.*, 1908) or $(1-C_{10}H_7)_3Bi$ (Arnauld *et al.*, 1999) to elemental tellurium has also been obtained by detelluration of $(1-C_{10}H_7)_2Te_2$, analogous to that of dimesityldítelluride (Akiba *et al.*, 1984). The angular geometry of $(1-C_{10}H_7)_2Te$ is quite similar to bis(*p*-substituted phenyl)tellurides (Farran *et al.*, 1997; Engman *et al.*, 2002) and the aromatic rings are oriented to give rise to nearly T-shaped conformation, presumably due to steric repulsion of 1-naphthyl units. However, the steric influence of the 1-naphthyl ligand on the molecular geometry of the title compound is neglibible when compared with the mesityl (Klapötke *et al.*, 2005), nonafluoromesityl (Voelker *et al.*, 1999) or supermesityl (Wieber *et al.*, 1995) analogues. The Te—C bond lengths and included angle compare well with the average values tabulated elsewhere (Allen, *et al.*, 1987; Allen *et al.*, 1993) and supramolecular associative η^6-$(1-C_{10}H_7)$···Te interactions observed in the crystal packing of $(1-C_{10}H_7)_2Te_2$ (Schulz Lang, *et al.*, 2002) are absent in the present case.

supplementary materials

Experimental

Compound (**I**) was serendipitously obtained on recrystallization of the reduction product of (1-$C_{10}H_7$)[(CH(Me)COC$_6$H$_5$)]TeCl$_2$ from dichloromethane. Detelluration of the corresponding ditelluride, (1-C$_{10}$H$_7$)$_2$Te$_2$ with metallic copper, analogous to that of dimesitylditelluride (Akiba *et al.*, 1984), also gave (**I**) in better yield.

Refinement

The H atoms were placed in geometrically calculated positions using a riding model (C—H$_{arom.}$ 0.95 Å) and the isotropic temperature factors constrained at 1.2 times U_{eq} of the carrier C atom. The maximum residual electron density of 1.048 e Å^3 is near the Te atom.

Figures
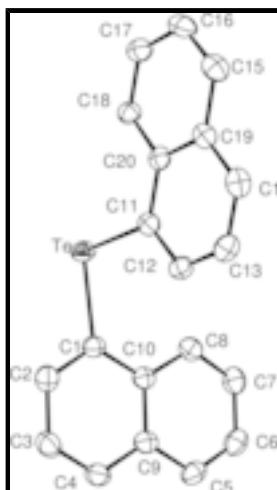
Fig. 1. The molecular structure of (**I**) showing 50% probability displacement ellipsoids and the atom numbering scheme.
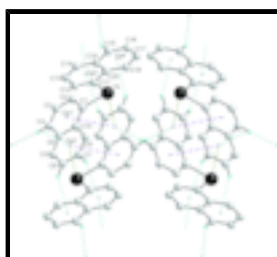
Fig. 2. The packing of (**I**) viewed along the *b* axis, showing pairs of molecules joined by reciprocal π···π interactions that are connected *via* C—H···π (ring centroid) interactions. H atoms not involved in the weak interactions have been omitted.

Bis(1-naphthyl) telluride

Crystal data

C$_{20}$H$_{14}$Te	$F_{000} = 1488$
$M_r = 381.91$	$D_x = 1.672$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo *Kα* radiation $\lambda = 0.71073$ Å

Hall symbol: -P 2ac 2ab

$a = 14.0662$ (6) Å

$b = 8.7390$ (4) Å

$c = 24.6881$ (11) Å

$V = 3034.8$ (2) Å^3

$Z = 8$

Cell parameters from 6102 reflections

$\theta = 2.9–27.5°$

$\mu = 1.95$ mm^{-1}

$T = 130$ (2) K

Block, yellow

$0.45 \times 0.40 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: sealed tube

Monochromator: graphite

$T = 130(2)$ K

φ and ω scans

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

$T_{min} = 0.460$, $T_{max} = 0.676$

11725 measured reflections

3477 independent reflections

3158 reflections with $I > 2\sigma(I)$

$R_{int} = 0.020$

$\theta_{max} = 27.5°$

$\theta_{min} = 1.7°$

$h = -11 \rightarrow 18$

$k = -11 \rightarrow 5$

$l = -28 \rightarrow 32$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.028$

$wR(F^2) = 0.073$

$S = 1.06$

3477 reflections

190 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 2.317P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 1.05$ e Å^{-3}

$\Delta\rho_{min} = -0.30$ e Å^{-3}

Extinction correction: none

Special details

Experimental. Characterization data for Compound (**I**) are: *M*.p. 108 ^{0}C [lit. 108 − 109 ^{0}C, Arnauld *et al.*, 1999; 126.5 ^{0}C, Lyons *et al.*, 1908];d ^{13}C (100.54 MHz, relative to Me$_4$Si in CDCl$_3$) 117.47, 126.29, 126.59, 126.96, 128.81, 129.19, 131.24, 133.76, 135.77, 137.97; d ^{125}Te (126.19 MHz, relative to Me$_2$Te, in CDCl$_3$) 466.5.

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 > 2sigma(F^2) is used only for calculat-

ing 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 ($Å^2$)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.45233 (17)	0.0854 (3)	0.42238 (10)	0.0245 (5)	
C2	0.40556 (19)	−0.0337 (3)	0.39838 (11)	0.0301 (5)	
H2	0.4267	−0.0706	0.3642	0.036*	
C3	0.32599 (19)	−0.1029 (3)	0.42369 (11)	0.0330 (6)	
H3	0.2948	−0.1866	0.4068	0.040*	
C4	0.29434 (18)	−0.0495 (3)	0.47212 (11)	0.0302 (5)	
H4	0.2401	−0.0950	0.4885	0.036*	
C5	0.31020 (18)	0.1264 (3)	0.54989 (10)	0.0299 (5)	
H5	0.2561	0.0810	0.5664	0.036*	
C6	0.35715 (19)	0.2418 (3)	0.57576 (10)	0.0320 (5)	
H6	0.3361	0.2755	0.6103	0.038*	
C7	0.4367 (2)	0.3111 (3)	0.55135 (11)	0.0320 (6)	
H7	0.4691	0.3914	0.5696	0.038*	
C8	0.46782 (18)	0.2640 (3)	0.50170 (10)	0.0280 (5)	
H8	0.5210	0.3131	0.4856	0.034*	
C9	0.34127 (17)	0.0736 (3)	0.49871 (10)	0.0252 (5)	
C10	0.42193 (16)	0.1426 (3)	0.47375 (10)	0.0231 (5)	
C11	0.50952 (17)	0.3739 (3)	0.35264 (9)	0.0226 (4)	
C12	0.41523 (16)	0.4055 (3)	0.36146 (10)	0.0245 (5)	
H12	0.3783	0.3376	0.3829	0.029*	
C13	0.37230 (17)	0.5371 (3)	0.33913 (10)	0.0273 (5)	
H13	0.3068	0.5567	0.3456	0.033*	
C14	0.42384 (17)	0.6364 (3)	0.30837 (10)	0.0280 (5)	
H14	0.3939	0.7239	0.2932	0.034*	
C15	0.57735 (18)	0.7114 (3)	0.26683 (10)	0.0289 (5)	
H15	0.5487	0.8003	0.2519	0.035*	
C16	0.67125 (19)	0.6829 (3)	0.25723 (10)	0.0310 (6)	
H16	0.7072	0.7512	0.2354	0.037*	
C17	0.71505 (18)	0.5523 (3)	0.27965 (10)	0.0283 (5)	
H17	0.7806	0.5334	0.2731	0.034*	
C18	0.66396 (17)	0.4529 (3)	0.31069 (9)	0.0239 (5)	
H18	0.6947	0.3658	0.3256	0.029*	
C19	0.52199 (17)	0.6101 (3)	0.29884 (9)	0.0238 (5)	
C20	0.56571 (16)	0.4768 (3)	0.32116 (9)	0.0222 (5)	
Te	0.574114 (11)	0.171144 (18)	0.382005 (6)	0.02580 (8)	
Cg1	0.3736	0.0192	0.4482	0.010*	0.00
Cg2	0.3892	0.1932	0.5252	0.010*	0.00
Cg3	0.4681	0.5066	0.3303	0.010*	0.00
Cg4	0.6192	0.5811	0.2891	0.010*	0.00

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0233 (11)	0.0249 (11)	0.0254 (12)	0.0004 (9)	0.0023 (9)	0.0034 (9)
C2	0.0315 (12)	0.0282 (13)	0.0306 (12)	0.0011 (10)	−0.0002 (11)	−0.0034 (10)
C3	0.0313 (13)	0.0277 (13)	0.0398 (14)	−0.0051 (11)	−0.0019 (11)	−0.0042 (11)
C4	0.0248 (12)	0.0273 (12)	0.0386 (14)	−0.0027 (10)	0.0026 (10)	0.0028 (10)
C5	0.0285 (12)	0.0325 (13)	0.0287 (12)	0.0051 (10)	0.0055 (10)	0.0064 (10)
C6	0.0350 (13)	0.0365 (14)	0.0246 (12)	0.0065 (11)	0.0016 (11)	−0.0007 (10)
C7	0.0382 (15)	0.0307 (13)	0.0272 (13)	0.0002 (10)	−0.0056 (11)	−0.0044 (10)
C8	0.0285 (12)	0.0270 (12)	0.0285 (12)	−0.0012 (10)	−0.0015 (10)	0.0015 (10)
C9	0.0241 (11)	0.0241 (11)	0.0274 (12)	0.0030 (9)	−0.0003 (9)	0.0076 (9)
C10	0.0236 (12)	0.0222 (11)	0.0235 (12)	0.0027 (9)	−0.0015 (9)	0.0054 (9)
C11	0.0271 (11)	0.0230 (10)	0.0176 (10)	−0.0014 (9)	−0.0020 (9)	−0.0007 (9)
C12	0.0237 (11)	0.0281 (12)	0.0218 (11)	−0.0006 (9)	0.0009 (9)	−0.0002 (9)
C13	0.0224 (11)	0.0336 (13)	0.0261 (12)	0.0040 (10)	−0.0027 (9)	−0.0029 (10)
C14	0.0312 (13)	0.0268 (12)	0.0261 (12)	0.0041 (10)	−0.0083 (10)	0.0001 (10)
C15	0.0352 (14)	0.0269 (12)	0.0247 (12)	−0.0007 (10)	−0.0068 (10)	0.0052 (10)
C16	0.0371 (15)	0.0288 (13)	0.0271 (12)	−0.0090 (10)	−0.0002 (11)	0.0065 (9)
C17	0.0254 (12)	0.0323 (13)	0.0273 (12)	−0.0029 (10)	0.0020 (10)	0.0000 (10)
C18	0.0255 (11)	0.0250 (11)	0.0213 (11)	0.0006 (9)	0.0004 (9)	0.0023 (9)
C19	0.0291 (12)	0.0234 (11)	0.0188 (10)	−0.0014 (10)	−0.0055 (9)	0.0002 (9)
C20	0.0254 (11)	0.0246 (11)	0.0168 (10)	−0.0006 (9)	−0.0026 (8)	−0.0029 (9)
Te	0.02321 (11)	0.02626 (11)	0.02792 (11)	0.00278 (6)	0.00458 (6)	0.00745 (6)

Geometric parameters (Å, °)

C1—C2	1.366 (4)	C11—C12	1.372 (3)
C1—C10	1.429 (3)	C11—C20	1.427 (3)
C1—Te	2.119 (2)	C11—Te	2.119 (2)
C2—C3	1.417 (4)	C12—C13	1.412 (3)
C2—H2	0.9500	C12—H12	0.9500
C3—C4	1.359 (4)	C13—C14	1.362 (4)
C3—H3	0.9500	C13—H13	0.9500
C4—C9	1.423 (3)	C14—C19	1.419 (3)
C4—H4	0.9500	C14—H14	0.9500
C5—C6	1.364 (4)	C15—C16	1.365 (4)
C5—C9	1.414 (3)	C15—C19	1.420 (3)
C5—H5	0.9500	C15—H15	0.9500
C6—C7	1.408 (4)	C16—C17	1.410 (4)
C6—H6	0.9500	C16—H16	0.9500
C7—C8	1.365 (4)	C17—C18	1.363 (3)
C7—H7	0.9500	C17—H17	0.9500
C8—C10	1.421 (4)	C18—C20	1.421 (3)
C8—H8	0.9500	C18—H18	0.9500
C9—C10	1.425 (3)	C19—C20	1.428 (3)
Cg1···Cg2^{i}	3.8752 (1)	Cg3···H15^{iii}	2.7238

Cg2···Te[i]	3.9567 (2)	Cg3···H7[iv]	2.7721
Cg2···H4[ii]	2.7485	Cg4···H6[iv]	2.8525
C2—C1—C10	120.5 (2)	C12—C11—Te	121.88 (18)
C2—C1—Te	117.04 (19)	C20—C11—Te	118.41 (17)
C10—C1—Te	122.39 (17)	C11—C12—C13	121.0 (2)
C1—C2—C3	120.9 (2)	C11—C12—H12	119.5
C1—C2—H2	119.5	C13—C12—H12	119.5
C3—C2—H2	119.5	C14—C13—C12	120.6 (2)
C4—C3—C2	120.0 (2)	C14—C13—H13	119.7
C4—C3—H3	120.0	C12—C13—H13	119.7
C2—C3—H3	120.0	C13—C14—C19	120.5 (2)
C3—C4—C9	120.9 (2)	C13—C14—H14	119.8
C3—C4—H4	119.5	C19—C14—H14	119.8
C9—C4—H4	119.5	C16—C15—C19	120.9 (2)
C6—C5—C9	120.7 (2)	C16—C15—H15	119.5
C6—C5—H5	119.7	C19—C15—H15	119.5
C9—C5—H5	119.7	C15—C16—C17	120.2 (2)
C5—C6—C7	120.2 (2)	C15—C16—H16	119.9
C5—C6—H6	119.9	C17—C16—H16	119.9
C7—C6—H6	119.9	C18—C17—C16	120.4 (2)
C8—C7—C6	120.6 (2)	C18—C17—H17	119.8
C8—C7—H7	119.7	C16—C17—H17	119.8
C6—C7—H7	119.7	C17—C18—C20	121.4 (2)
C7—C8—C10	121.1 (2)	C17—C18—H18	119.3
C7—C8—H8	119.5	C20—C18—H18	119.3
C10—C8—H8	119.5	C14—C19—C15	121.7 (2)
C5—C9—C4	121.0 (2)	C14—C19—C20	119.2 (2)
C5—C9—C10	119.6 (2)	C15—C19—C20	119.2 (2)
C4—C9—C10	119.3 (2)	C18—C20—C11	123.0 (2)
C8—C10—C9	117.9 (2)	C18—C20—C19	118.0 (2)
C8—C10—C1	123.8 (2)	C11—C20—C19	119.1 (2)
C9—C10—C1	118.3 (2)	C1—Te—C11	96.32 (9)
C12—C11—C20	119.7 (2)	H15[iii]—Cg3—H7[iv]	154.7
C10—C1—C2—C3	0.1 (4)	C11—C12—C13—C14	−0.2 (4)
Te—C1—C2—C3	177.1 (2)	C12—C13—C14—C19	−0.8 (4)
C1—C2—C3—C4	1.0 (4)	C19—C15—C16—C17	−0.7 (4)
C2—C3—C4—C9	−1.4 (4)	C15—C16—C17—C18	0.5 (4)
C9—C5—C6—C7	0.7 (4)	C16—C17—C18—C20	0.3 (4)
C5—C6—C7—C8	0.0 (4)	C13—C14—C19—C15	179.8 (2)
C6—C7—C8—C10	−1.0 (4)	C13—C14—C19—C20	1.0 (4)
C6—C5—C9—C4	178.3 (2)	C16—C15—C19—C14	−178.8 (2)
C6—C5—C9—C10	−0.5 (4)	C16—C15—C19—C20	0.0 (4)
C3—C4—C9—C5	−178.1 (2)	C17—C18—C20—C11	178.8 (2)
C3—C4—C9—C10	0.7 (4)	C17—C18—C20—C19	−1.0 (3)
C7—C8—C10—C9	1.2 (4)	C12—C11—C20—C18	179.4 (2)
C7—C8—C10—C1	−178.4 (2)	Te—C11—C20—C18	−2.9 (3)
C5—C9—C10—C8	−0.4 (3)	C12—C11—C20—C19	−0.8 (3)
C4—C9—C10—C8	−179.2 (2)	Te—C11—C20—C19	176.93 (16)

C5—C9—C10—C1	179.2 (2)	C14—C19—C20—C18	179.6 (2)
C4—C9—C10—C1	0.4 (3)	C15—C19—C20—C18	0.8 (3)
C2—C1—C10—C8	178.8 (2)	C14—C19—C20—C11	−0.2 (3)
Te—C1—C10—C8	2.0 (3)	C15—C19—C20—C11	−179.0 (2)
C2—C1—C10—C9	−0.8 (3)	C2—C1—Te—C11	105.2 (2)
Te—C1—C10—C9	−177.60 (16)	C10—C1—Te—C11	−77.9 (2)
C20—C11—C12—C13	1.0 (4)	C12—C11—Te—C1	−2.4 (2)
Te—C11—C12—C13	−176.60 (18)	C20—C11—Te—C1	179.90 (17)

Symmetry codes: (i) −x+1, −y, −z+1; (ii) −x+1/2, y+1/2, z; (iii) −x+1, y−1/2, −z+1/2; (iv) −x+1, −y+1, −z+1.

Fig. 1

Fig. 2