



IUCrData

ISSN 2414-3146

Received 13 December 2023

Accepted 14 December 2023

Edited by W. T. A. Harrison, University of  
Aberdeen, United Kingdom

**Keywords:** tellurium; heterocyclic;  
organotellurium; oxatellurole; crystal structure.

CCDC reference: 2314478

**Structural data:** full structural data are available  
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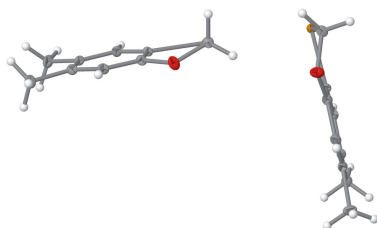
## 5,6-Dimethylbenzo[*d*][1,3]oxatellurole

Samantha Ponzo,<sup>a</sup> Alanna Turner,<sup>a</sup> Frank R. Fronczek<sup>b</sup> and Thomas Junk<sup>a\*</sup>

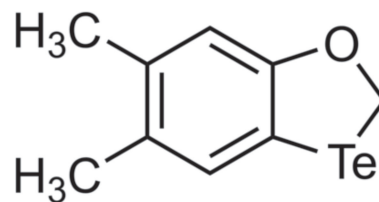
<sup>a</sup>Department of Chemistry, Lafayette, LA 70403, USA, and <sup>b</sup>Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803, USA. \*Correspondence e-mail: [thomas.junk@louisiana.edu](mailto:thomas.junk@louisiana.edu)

The structure of the title compound, C<sub>9</sub>H<sub>10</sub>OTe, at 100 K has orthorhombic (*P*2<sub>1</sub>2<sub>1</sub>2) symmetry with two independent molecules in the asymmetric unit (*Z'* = 2). The molecules are folded along their Te...O axes, with their Te–C–O planes angled at an average of 25.1° with respect to the remaining non-H atoms, which are almost coplanar (average deviation from planarity = 0.04 Å). A Hirshfeld plot shows weak intermolecular interactions between the two Te atoms located in each asymmetric molecule, with a Te...Te distance of 3.7191 (4) Å. The structure is strongly pseudosymmetric to the space group *Pccn* with *Z'* = 1. The crystal chosen for data collection was found to be an inversion twin.

### 3D view



### Chemical scheme



### Structure description

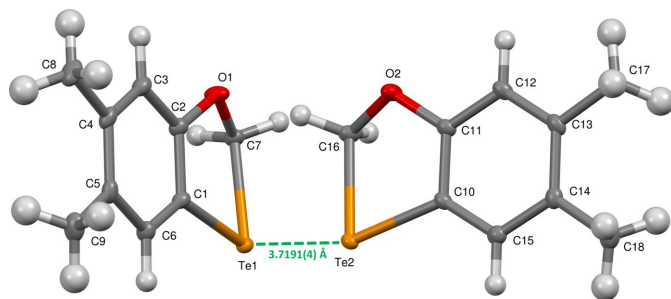
Tellurium/oxygen-containing heterocycles have received significant attention as potent enzyme inhibitors and antioxidants. Thus, organotelluroxetanes inhibit cysteine proteases (Persike *et al.*, 2008) while derivatives of 1,3,2-dioxatellurothane inhibit IL-1  $\beta$  converting enzyme (Brodsky *et al.*, 2007; Ba *et al.*, 2010) and proteases (Albeck *et al.*, 1998). Derivatives of [1,2]oxatellurole act as glutathione peroxidase mimetics (Back *et al.*, 2005) while octa-*O*-bis-(*R,R*)-tartarate ditellurane ('SAS') provides pro-apoptotic signaling in drug-resistant multiple myeloma (Zigman-Hoffman *et al.*, 2021). [1,4]Oxatelluranes have been known for over seventy years (Farrar & Gulland, 1945). In contrast, [1,3]oxatelluroles have remained unknown, making the title compound, 5,6-dimethylbenzo[*d*][1,3]oxatellurole, C<sub>9</sub>H<sub>10</sub>OTe, the first member of this class: the two molecules in the asymmetric unit are shown in Fig. 1.

Furthermore, a search of the Cambridge Structural Database (May 2021 update; Groom *et al.*, 2016) for [1,3]oxaselenoles and [1,3]oxathioles indicates a paucity of such structures as well. One [1,3]oxaselenole (Laitalainen *et al.*, 1983) and thirteen sulfur congeners are known, such as the structurally similar 6,6-dimethyl-[1,3]dioxolo[4',5':4,5]-benzo[1,2-*d*][1,3]oxathiole-8-carbaldehyde (Wessig *et al.*, 2021). Reported derivatives of selenafulvalene and tetratellurafulvalene (Kojima *et al.*, 2004; Carroll *et al.*, 1982) bear only limited structural resemblance to the title compound, since these molecules are



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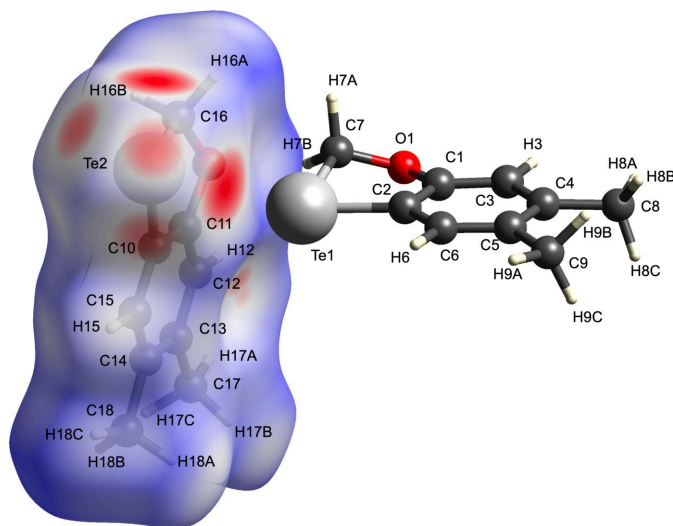
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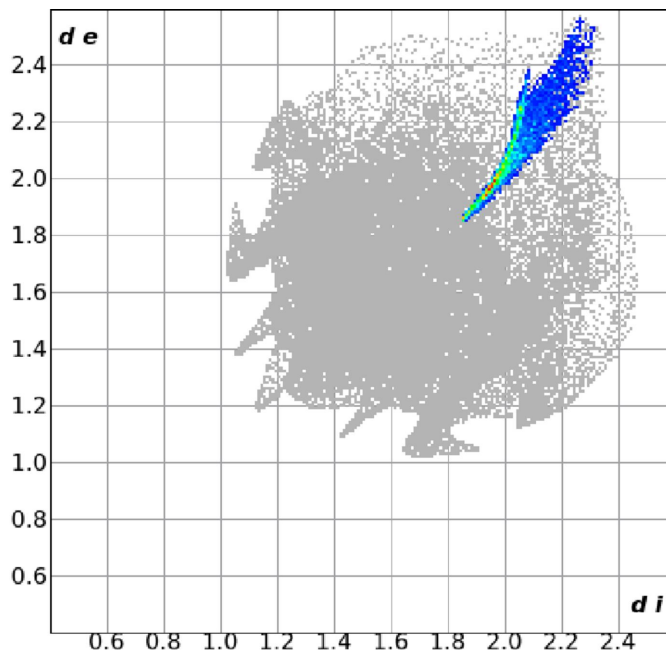
**Figure 1**  
The asymmetric unit of the title compound with 50% displacement ellipsoids.

almost planar due to the absence of an  $sp^3$ -hybridized carbon atom in the heteroaromatic ring. The non-planarity in the title compound accommodates near-tetrahedral angles at the bridging carbon atom [ $\text{Te1}-\text{C7}-\text{O1} = 108.27(19)^\circ$ ,  $\text{Te2}-\text{C16}-\text{O2} = 108.16(19)^\circ$ ] for the two independent molecules; the  $\text{C1}-\text{Te1}-\text{C7}$  and  $\text{C10}-\text{Te2}-\text{C16}$  angles are  $78.40(11)$  and  $78.24(11)^\circ$ , respectively.

The Hirshfeld surface enclosing each of the two independent molecules was calculated with respect to  $d_e$ ,  $d_i$  and  $d_{\text{norm}}$  using the *Crystal Explorer* program (Spackman *et al.*, 2021), where  $d_e$  and  $d_i$  represent the nearest distance of external or internal nucleus from a point of interest on the iso-surface. The surfaces of both independent molecules are nearly identical, indicating interactions as bright-red areas on the Hirshfeld surface as shown in Fig. 2. The strongest of these corresponds to the  $\text{Te1} \cdots \text{Te2}$  close contact of  $3.7191(4)$  Å between the tellurium atoms in the two independent molecules (Fig. 1). This compares to  $2.7072(9)$  Å for the representative covalent  $\text{Te}-\text{Te}$  bond of diphenyl ditelluride (Fuller *et al.*, 2010), indicating a relatively weak interaction. A two-dimensional fingerprint plot highlighting the reciprocal  $\text{Te} \cdots \text{Te}$  contact is shown in Fig. 3: it accounts for 8.8% of the surface area.



**Figure 2**  
The Hirshfeld surface of the title compound mapped over  $d_{\text{norm}}$ .



**Figure 3**  
Two-dimensional fingerprint plot showing the region corresponding to intermolecular  $\text{Te} \cdots \text{Te}$  contacts in red.

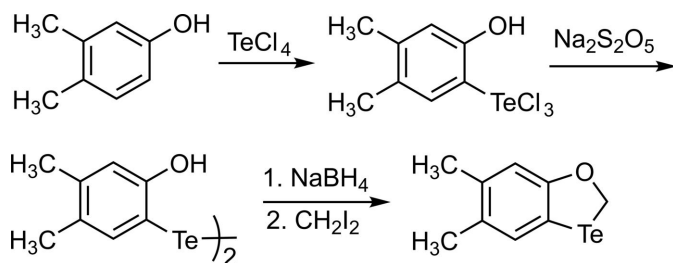
*checkCIF* (Spek, 2020) reports a 100% fit for an inversion center in the title structure and suggests space group *Pccn*. Indeed, the structure can be solved and refined in *Pccn* with  $Z' = 1$ , but the  $R(F)$  value is 0.18, the ellipsoids are elongated, and there are numerous violations of all three glide-plane absence conditions. The  $P2_12_12$  refinement yields a local center at  $0.740, 0.758, 0.749$ , offset from the position necessary for *Pccn*, so it is clear that this is a case of the ‘inverse Marsh’ situation (Fronczek, 2018), where the structure can be approximately described in a space group of too high symmetry.

## Synthesis and crystallization

The title compound was prepared in three steps, starting with 3,4-dimethylphenol and tellurium tetrachloride as outlined in Fig. 4.

**2-Hydroxy-3,4-dimethyltellurium trichloride:** A 100 ml round-bottom flask with magnetic stirring, reflux condenser and drying tube was charged with tellurium tetrachloride (4.31 g, 16 mmol), 3,4-dimethylphenol (1.95 g, 16 mmol) and dry toluene (8 ml). The mixture was stirred and heated to reflux for 45 min. A color change to dark yellow was observed. The clear solution was decanted from solids (mostly tellurium) while still hot and allowed to cool. The resulting product was collected by filtration. Yellow crystals, 2.77 g (49%). The product was pure enough for further use. An analytical sample was obtained by recrystallization from acetonitrile, m.p.  $174-175^\circ\text{C}$ ,  $^1\text{H}$  NMR ( $\text{DMSO}-d_6$ , p.p.m.): 2.18 (s, 3H); 2.21 (s, 3H) 6.78 (s, 1H), 7.62 (s, 1H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , p.p.m.): 18.68, 19.53, 117.00, 128.44, 130.70, 141.85, 154.33.

**Bis(2-hydroxy-4,5-dimethylphenyl) ditelluride:** A 100 ml round-bottom flask with magnetic stirring was charged with



**Figure 4**  
Synthesis of the title compound.

2-hydroxy-3,4-dimethyltellurium trichloride (2.13 g, 6 mmol), sodium metabisulfite (3.42 g, 18 mmol), 95% ethanol (2 ml), water (10 ml) and dichloromethane (10 ml). The mixture was stirred for 5 min, during which time it turned dark red. It was subjected to centrifugation to achieve phase separation. The organic phase was collected with a pipette and the solvent evaporated as quickly as feasible under reduced pressure. Red solid, 0.72 g (48%), mp  $\sim 310^\circ\text{C}$  (decomposition). The product is stable in solid form but decomposes rapidly in solution with tellurium formation. Consequently, it was not characterized by NMR spectroscopy.

**5,6-Dimethylbenzo[d][1,3]oxatellurole:** A 50 ml round-bottom flask with magnetic stirring, reflux condenser and nitrogen purge line was charged with bis(2-hydroxy-4,5-dimethylphenyl) ditelluride (0.24 g, 0.5 mmol) and 95% ethanol (5 ml). The mixture was purged with nitrogen and excess sodium borohydride was added (80 mg, 2 mmol). The mixture was stirred for 5 min, then brought to reflux for 2 min to assure complete reduction. Diiodomethane was added (0.2 g, 0.75 mmol) and heating resumed for another 5 min, resulting in a color change to yellow. The product subsequently precipitated after addition of water (15 ml) and was collected by centrifugation. It was taken up in chloroform (5 ml), the solution centrifuged to remove traces of solids and the product crystallized by concentration to approx. 1 ml volume. Yellow needles, 61 mg (23%), m.p.  $159\text{--}160^\circ\text{C}$ . Like other mono-tellurides, the product is prone to slow oxidation in solution in solution. A crystal suitable for X-ray crystallography was obtained by concentration of a solution in chloroform.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , p.p.m.): 2.16 (s, 3H), 2.22 (s, 3H), 6.35 (s, 2H), 6.632 (s, 1H), 7.009 (s, 1H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , p.p.m.): 19.04, 19.64, 51.11, 101.94, 112.81, 131.32, 132.93, 136.67, 159.58.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The Flack parameter (Flack & Bernardinelli, 2000) refined to 0.49 (4), indicative of an inversion twin.

## Acknowledgements

We are grateful to the Department of Chemistry, University of Louisiana at Lafayette for material support of this work.

**Table 1**  
Experimental details.

Crystal data	
Chemical formula	$\text{C}_9\text{H}_{10}\text{OTe}$
$M_r$	261.77
Crystal system, space group	Orthorhombic, $P2_12_12$
Temperature (K)	100
$a, b, c$ (Å)	13.6947 (12), 23.467 (2), 5.2287 (6)
$V$ (Å <sup>3</sup> )	1680.3 (3)
$Z$	8
Radiation type	Ag $K\alpha$ , $\lambda = 0.56086$ Å
$\mu$ (mm <sup>-1</sup> )	1.84
Crystal size (mm)	$0.23 \times 0.10 \times 0.09$
Data collection	
Diffraction	Bruker D8 Venture DUO with Photon III C14
Absorption correction	Multi-scan (SADABS; Krause <i>et al.</i> , 2015)
$T_{\min}, T_{\max}$	0.701, 0.852
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	83209, 11161, 9763
$R_{\text{int}}$	0.080
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.926
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.033, 0.061, 1.05
No. of reflections	11161
No. of parameters	204
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	1.74, -1.28
Absolute structure	Refined as an inversion twin.
Absolute structure parameter	0.49 (4)

Computer programs: APEX4 and SAINT (Bruker, 2016), SHELXT2018/2 (Sheldrick, 2015), SHELXL2018/1 (Sheldrick, 2015), Mercury (Macrae *et al.*, 2020), and publCIF (Westrip, 2010).

## Funding information

Funding for this research was provided by: Louisiana Board of Regents (grant No. LEQSF(2011-12)-ENH-TR-01).

## References

- Albeck, A., Weitman, H., Sredni, B. & Albeck, M. (1998). *Inorg. Chem.* **37**, 1704–1712.
- Ba, L. A., Döring, M., Jamier, V. & Jacob, C. (2010). *Org. Biomol. Chem.* **8**, 4203–4216.
- Back, T. G., Kuzma, D. & Parvez, M. (2005). *J. Org. Chem.* **70**, 9230–9236.
- Brodsky, M., Yosef, S., Galit, R., Albeck, M., Longo, D. L., Albeck, A. & Sredni, B. (2007). *J. Interferon Cytokine Res.* **27**, 453–462.
- Bruker (2016). APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
- Carroll, P. J., Lakshmikantham, M. V., Cave, M. P., Wudl, F., Aharon-Shalom, E. & Cox, S. D. (1982). *J. Chem. Soc. Chem. Commun.* pp. 1316–1318.
- Farrar, W. V. & Gulland, J. M. (1945). *J. Chem. Soc.* pp. 11–14.
- Flack, H. D. & Bernardinelli, G. (2000). *J. Appl. Cryst.* **33**, 1143–1148.
- Fronczek, F. R. (2018). *Acta Cryst.* **A74**, a60.
- Fuller, A. L., Scott-Hayward, L. A. S., Li, Y., Bühl, M., Slawin, A. M. Z. & Woollins, J. D. (2010). *J. Am. Chem. Soc.* **132**, 5799–5802.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Kojima, T., Tanaka, K., Ishida, T. & Nogami, T. (2004). *J. Org. Chem.* **69**, 9319–9322.

- Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
- Laitalainen, T., Simonen, T., Kivekäs, R. & Klinga, M. (1983). *J. Chem. Soc. Perkin Trans. 1*, pp. 333–340.
- Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
- Persike, D. S., Cunha, R. L. O. R., Juliano, L., Silva, I. R., Rosim, F. E., Vignoli, T., Dona, F., Cavaleiro, E. A. & Fernandes, M. J. da S. (2008). *Neurobiol. Dis.* **31**, 120–126.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.
- Spek, A. L. (2020). *Acta Cryst.* **E76**, 1–11.
- Wessig, P., John, L., Sperlich, E. & Kelling, A. (2021). *Eur. J. Org. Chem.* pp. 499–511.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
- Zigman-Hoffman, E., Sredni, B., Meilik, B., Naparstek, E. & Tartakovsky, B. (2021). *Leuk. Lymphoma*, **62**, 1146–1156.

## full crystallographic data

*IUCrData* (2024). **9**, x231076 [<https://doi.org/10.1107/S2414314623010763>]

## 5,6-Dimethylbenzo[d][1,3]oxatellurole

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*Crystal data*

$\text{C}_9\text{H}_{10}\text{OTe}$	$D_x = 2.069 \text{ Mg m}^{-3}$
$M_r = 261.77$	Ag $K\alpha$ radiation, $\lambda = 0.56086 \text{ \AA}$
Orthorhombic, $P2_12_12$	Cell parameters from 9865 reflections
$a = 13.6947 (12) \text{ \AA}$	$\theta = 2.4\text{--}30.8^\circ$
$b = 23.467 (2) \text{ \AA}$	$\mu = 1.84 \text{ mm}^{-1}$
$c = 5.2287 (6) \text{ \AA}$	$T = 100 \text{ K}$
$V = 1680.3 (3) \text{ \AA}^3$	Needle, yellow
$Z = 8$	$0.23 \times 0.10 \times 0.09 \text{ mm}$
$F(000) = 992$	

*Data collection*

Bruker D8 Venture DUO with Photon III C14 diffractometer	11161 independent reflections
Radiation source: $\text{I}\mu\text{S}$ 3.0 microfocus	9763 reflections with $I > 2\sigma(I)$
$\varphi$ and $\omega$ scans	$R_{\text{int}} = 0.080$
Absorption correction: multi-scan (SADABS; Krause <i>et al.</i> , 2015)	$\theta_{\text{max}} = 31.3^\circ$ , $\theta_{\text{min}} = 2.4^\circ$
$T_{\text{min}} = 0.701$ , $T_{\text{max}} = 0.852$	$h = -23 \rightarrow 25$
83209 measured reflections	$k = -43 \rightarrow 43$
	$l = -9 \rightarrow 9$

*Refinement*

Refinement on $F^2$	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0081P)^2 + 1.4627P]$
$R[F^2 > 2\sigma(F^2)] = 0.033$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.061$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.05$	$\Delta\rho_{\text{max}} = 1.74 \text{ e \AA}^{-3}$
11161 reflections	$\Delta\rho_{\text{min}} = -1.28 \text{ e \AA}^{-3}$
204 parameters	Absolute structure: Refined as an inversion twin.
0 restraints	Absolute structure parameter: 0.49 (4)
Hydrogen site location: inferred from neighbouring sites	

*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.** Refined as a 2-component inversion twin.

All H atoms were located in difference maps and then treated as riding in geometrically idealized positions with C—H distances  $0.95 \text{ \AA}$  and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$  for the attached C atom ( $0.98 \text{ \AA}$  and  $1.5U_{\text{eq}}$  for methyl groups).

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Te1	0.60109 (2)	0.44282 (2)	0.70610 (4)	0.01156 (3)
O1	0.66046 (16)	0.32225 (8)	0.7300 (5)	0.0171 (4)
C1	0.7160 (2)	0.40889 (11)	0.9272 (6)	0.0125 (5)
C2	0.7249 (2)	0.35032 (12)	0.8897 (6)	0.0139 (5)
C3	0.7937 (2)	0.31871 (13)	1.0236 (6)	0.0157 (5)
H3	0.799879	0.278965	0.993125	0.019*
C4	0.8534 (2)	0.34532 (12)	1.2023 (8)	0.0165 (5)
C5	0.8459 (2)	0.40437 (13)	1.2423 (6)	0.0156 (6)
C6	0.7776 (2)	0.43536 (13)	1.1010 (6)	0.0146 (5)
H6	0.773282	0.475424	1.124329	0.018*
C7	0.6149 (2)	0.35744 (11)	0.5459 (6)	0.0139 (5)
H7A	0.549569	0.342150	0.502599	0.017*
H7B	0.654591	0.358629	0.387739	0.017*
C8	0.9241 (2)	0.31015 (15)	1.3595 (7)	0.0229 (7)
H8A	0.926472	0.271228	1.291820	0.034*
H8B	0.902188	0.309218	1.537911	0.034*
H8C	0.989287	0.327225	1.350549	0.034*
C9	0.9089 (2)	0.43445 (15)	1.4362 (7)	0.0227 (6)
H9A	0.901315	0.475753	1.416802	0.034*
H9B	0.977412	0.424028	1.408941	0.034*
H9C	0.888931	0.423143	1.608829	0.034*
Te2	0.40868 (2)	0.43608 (2)	0.20506 (4)	0.01157 (3)
O2	0.36896 (16)	0.31277 (8)	0.2343 (5)	0.0164 (4)
C10	0.2997 (2)	0.39623 (11)	0.4274 (6)	0.0123 (5)
C11	0.3004 (2)	0.33735 (11)	0.3916 (6)	0.0134 (5)
C12	0.2362 (2)	0.30266 (12)	0.5262 (6)	0.0144 (5)
H12	0.236775	0.262634	0.499077	0.017*
C13	0.1713 (2)	0.32627 (12)	0.6998 (7)	0.0151 (5)
C14	0.1696 (2)	0.38537 (12)	0.7403 (6)	0.0143 (5)
C15	0.2342 (2)	0.41978 (12)	0.5996 (7)	0.0150 (5)
H15	0.232865	0.459917	0.622981	0.018*
C16	0.4082 (2)	0.35010 (11)	0.0473 (6)	0.0146 (5)
H16A	0.367958	0.348854	−0.109910	0.018*
H16B	0.475554	0.338379	0.002856	0.018*
C17	0.1054 (3)	0.28707 (14)	0.8522 (7)	0.0213 (6)
H17A	0.110824	0.248173	0.785524	0.032*
H17B	0.037659	0.300080	0.837329	0.032*
H17C	0.125151	0.287618	1.032360	0.032*
C18	0.1027 (2)	0.41186 (15)	0.9348 (7)	0.0202 (6)
H18A	0.126438	0.403030	1.107197	0.030*
H18B	0.036663	0.396560	0.913427	0.030*
H18C	0.101551	0.453273	0.910780	0.030*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Te1	0.01223 (6)	0.00991 (5)	0.01252 (8)	0.00161 (5)	0.00064 (7)	0.00114 (6)
O1	0.0230 (10)	0.0110 (7)	0.0173 (12)	0.0028 (7)	−0.0044 (9)	−0.0001 (8)
C1	0.0140 (12)	0.0119 (10)	0.0115 (13)	0.0022 (9)	0.0008 (10)	0.0007 (9)
C2	0.0156 (12)	0.0142 (10)	0.0118 (12)	0.0023 (9)	0.0008 (10)	−0.0006 (9)
C3	0.0158 (12)	0.0157 (11)	0.0155 (14)	0.0036 (10)	0.0017 (11)	0.0022 (10)
C4	0.0137 (11)	0.0210 (11)	0.0147 (12)	0.0054 (9)	0.0022 (13)	0.0019 (13)
C5	0.0114 (10)	0.0239 (12)	0.0116 (15)	0.0003 (9)	0.0012 (9)	−0.0007 (9)
C6	0.0143 (11)	0.0168 (11)	0.0127 (12)	0.0006 (10)	−0.0004 (10)	−0.0021 (10)
C7	0.0161 (12)	0.0120 (10)	0.0136 (13)	0.0007 (9)	−0.0008 (10)	−0.0023 (9)
C8	0.0173 (14)	0.0296 (15)	0.0219 (17)	0.0074 (12)	−0.0014 (12)	0.0063 (13)
C9	0.0157 (12)	0.0352 (16)	0.0172 (15)	−0.0019 (14)	−0.0029 (11)	−0.0050 (13)
Te2	0.01233 (7)	0.01001 (6)	0.01239 (8)	−0.00127 (5)	−0.00103 (7)	0.00133 (6)
O2	0.0214 (9)	0.0116 (7)	0.0160 (12)	−0.0015 (7)	0.0048 (9)	−0.0006 (7)
C10	0.0132 (11)	0.0122 (10)	0.0114 (12)	−0.0020 (9)	−0.0005 (9)	0.0012 (9)
C11	0.0153 (12)	0.0122 (10)	0.0126 (12)	−0.0020 (9)	−0.0014 (10)	−0.0008 (9)
C12	0.0173 (13)	0.0140 (10)	0.0121 (13)	−0.0037 (9)	−0.0016 (11)	−0.0001 (9)
C13	0.0143 (10)	0.0174 (10)	0.0135 (12)	−0.0052 (8)	−0.0034 (12)	0.0010 (12)
C14	0.0121 (10)	0.0194 (11)	0.0115 (15)	0.0001 (9)	−0.0007 (9)	−0.0001 (9)
C15	0.0141 (12)	0.0151 (11)	0.0157 (14)	0.0001 (9)	−0.0022 (11)	−0.0011 (10)
C16	0.0189 (13)	0.0120 (9)	0.0130 (13)	−0.0009 (10)	−0.0008 (11)	−0.0021 (8)
C17	0.0200 (14)	0.0238 (13)	0.0201 (17)	−0.0080 (12)	0.0031 (12)	0.0034 (11)
C18	0.0164 (13)	0.0287 (14)	0.0157 (15)	0.0001 (12)	0.0003 (12)	−0.0025 (11)

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

Te1—C1	2.108 (3)	Te2—C10	2.110 (3)
Te1—C7	2.180 (3)	Te2—C16	2.180 (3)
O1—C2	1.382 (4)	O2—C11	1.375 (4)
O1—C7	1.414 (4)	O2—C16	1.419 (4)
C1—C6	1.387 (4)	C10—C15	1.387 (4)
C1—C2	1.394 (4)	C10—C11	1.394 (4)
C2—C3	1.388 (4)	C11—C12	1.390 (4)
C3—C4	1.390 (5)	C12—C13	1.386 (5)
C3—H3	0.9500	C12—H12	0.9500
C4—C5	1.405 (4)	C13—C14	1.403 (4)
C4—C8	1.514 (4)	C13—C17	1.515 (4)
C5—C6	1.396 (4)	C14—C15	1.405 (4)
C5—C9	1.506 (4)	C14—C18	1.503 (4)
C6—H6	0.9500	C15—H15	0.9500
C7—H7A	0.9900	C16—H16A	0.9900
C7—H7B	0.9900	C16—H16B	0.9900
C8—H8A	0.9800	C17—H17A	0.9800
C8—H8B	0.9800	C17—H17B	0.9800
C8—H8C	0.9800	C17—H17C	0.9800
C9—H9A	0.9800	C18—H18A	0.9800

C9—H9B	0.9800	C18—H18B	0.9800
C9—H9C	0.9800	C18—H18C	0.9800
C1—Te1—C7	78.40 (11)	C10—Te2—C16	78.24 (11)
C2—O1—C7	114.5 (2)	C11—O2—C16	114.3 (2)
C6—C1—C2	118.7 (3)	C15—C10—C11	119.1 (3)
C6—C1—Te1	130.1 (2)	C15—C10—Te2	129.7 (2)
C2—C1—Te1	111.2 (2)	C11—C10—Te2	111.1 (2)
O1—C2—C3	118.9 (2)	O2—C11—C12	119.3 (2)
O1—C2—C1	119.9 (3)	O2—C11—C10	120.0 (3)
C3—C2—C1	121.0 (3)	C12—C11—C10	120.6 (3)
C2—C3—C4	119.9 (3)	C13—C12—C11	120.2 (3)
C2—C3—H3	120.1	C13—C12—H12	119.9
C4—C3—H3	120.1	C11—C12—H12	119.9
C3—C4—C5	120.0 (3)	C12—C13—C14	120.3 (3)
C3—C4—C8	119.7 (3)	C12—C13—C17	118.9 (3)
C5—C4—C8	120.2 (3)	C14—C13—C17	120.7 (3)
C6—C5—C4	118.9 (3)	C13—C14—C15	118.6 (3)
C6—C5—C9	119.7 (3)	C13—C14—C18	121.4 (3)
C4—C5—C9	121.4 (3)	C15—C14—C18	120.0 (3)
C1—C6—C5	121.4 (3)	C10—C15—C14	121.2 (3)
C1—C6—H6	119.3	C10—C15—H15	119.4
C5—C6—H6	119.3	C14—C15—H15	119.4
O1—C7—Te1	108.27 (19)	O2—C16—Te2	108.16 (19)
O1—C7—H7A	110.0	O2—C16—H16A	110.1
Te1—C7—H7A	110.0	Te2—C16—H16A	110.1
O1—C7—H7B	110.0	O2—C16—H16B	110.1
Te1—C7—H7B	110.0	Te2—C16—H16B	110.1
H7A—C7—H7B	108.4	H16A—C16—H16B	108.4
C4—C8—H8A	109.5	C13—C17—H17A	109.5
C4—C8—H8B	109.5	C13—C17—H17B	109.5
H8A—C8—H8B	109.5	H17A—C17—H17B	109.5
C4—C8—H8C	109.5	C13—C17—H17C	109.5
H8A—C8—H8C	109.5	H17A—C17—H17C	109.5
H8B—C8—H8C	109.5	H17B—C17—H17C	109.5
C5—C9—H9A	109.5	C14—C18—H18A	109.5
C5—C9—H9B	109.5	C14—C18—H18B	109.5
H9A—C9—H9B	109.5	H18A—C18—H18B	109.5
C5—C9—H9C	109.5	C14—C18—H18C	109.5
H9A—C9—H9C	109.5	H18A—C18—H18C	109.5
H9B—C9—H9C	109.5	H18B—C18—H18C	109.5