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Dibromodiphenyltellurium(IV)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.008 Å
R factor = 0.029
wR factor = 0.070
Data-to-parameter ratio = 20.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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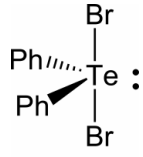
The previously described structure of diphenyltellurium dibromide, $C_{12}H_{10}Br_2Te$, has been reinvestigated. The molecule lies on a twofold rotation axis.

Comment

The supramolecular structures of diorganotellurium dihalides, R_2TeX_2 (R = alkyl, aryl; X = F, Cl, Br, I), which have been analysed using the concepts of crystal engineering, have attracted great attention in recent years due to their diverse modes of secondary interactions (Zukerman-Schpector & Haiduc, 2001). We have now reinvestigated the structure of diphenyltellurium dibromide, first described without inclusion of H atoms (Christofferson & McCullough, 1958) for comparison with similar compounds prepared by our group (Beckmann *et al.*, 2004). The molecule lies on a twofold rotation axis. Unlike the recently investigated $(Me_2NC_6H_4)_2TeBr_2$ (Beckmann *et al.*, 2004), which shows secondary Br···Br, but no Te···Br interactions, Ph_2TeBr_2 reveals two secondary Te···Br interactions (Fig. 1).



(I)

Experimental

The title compound was prepared according to the original literature procedure (Krafft & Lyons, 1894)

Crystal data

$C_{12}H_{10}Br_2Te$
M_r = 441.62
Tetragonal, $I4_1$
a = 11.4345 (7) Å
c = 9.8068 (12) Å
V = 1282.22 (19) Å^3
Z = 4
D_x = 2.288 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2187 reflections
θ = 2.5–27.4°
μ = 8.52 mm^{-1}
T = 295 (2) K
Block, yellow
0.40 × 0.35 × 0.35 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.043, T_{max} = 0.050
3889 measured reflections
1419 independent reflections
1323 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.4°
h = −14 → 8
k = −14 → 14
l = −12 → 12

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.029$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.070$	$\Delta\rho_{max} = 0.74$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.31$ e Å^{-3}
1419 reflections	Absolute structure: Flack (1983)
69 parameters	Flack parameter = 0.069 (16)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Te—Br	2.6818 (6)	Te—C1	2.133 (5)
Br—Te—Br^{i}	177.31 (3)	C1^{i}—Te—Br	91.36 (12)
C1—Te—Br	90.42 (12)	C1^{i}—Te—C1	96.9 (3)

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

The H atoms were placed in geometrically calculated positions and refined using a riding model (C—H = 0.93 Å). The isotropic displacement parameters were constrained at $1.2U_{eq}$(C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Bergerhoff *et al.*, 1996); software used to prepare material for publication: *SHELXL*97.

Dr Jonathan White (The University of Melbourne) is gratefully acknowledged for the X-ray data collection.

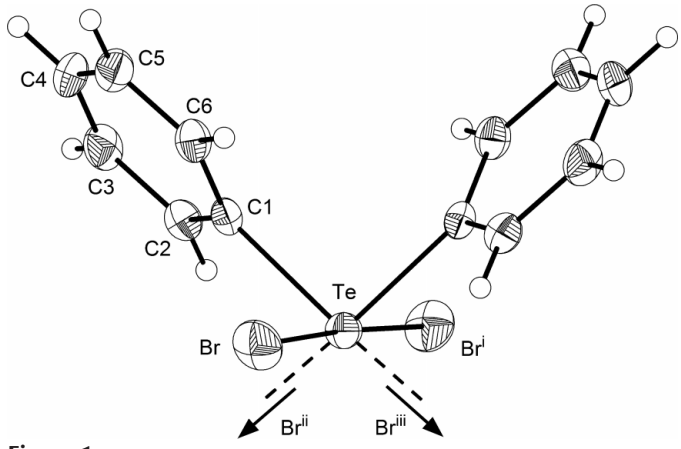


Figure 1
View of (I), showing the labelling of non-H atoms. Displacement ellipsoids are shown at 30% probability levels. [Symmetry codes: (i) $-x$, $1-y$, z; (ii) $\frac{1}{2}-y$, x, $z-\frac{1}{4}$, (iii) $y-\frac{1}{2}$, $1-x$, $z-\frac{1}{4}$.]

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