

2,4,6-Tri-*tert*-butylbenzenetellurenyl iodide

Thomas M. Klapötke,* Burkhard Krumm and Ingo Schwab

Department of Chemistry and Biochemistry,
Ludwig-Maximilian University, Butenandtstrasse
5–13 (Haus D), D-81377 Munich, GermanyCorrespondence e-mail:
tmk@cup.uni-muenchen.de

Key indicators

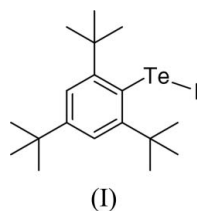
Single-crystal X-ray study
 $T = 200\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.026
 wR factor = 0.062
Data-to-parameter ratio = 19.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The crystal structure of Mes^*TeI ($\text{Mes}^* = 2,4,6\text{-tri-}i\text{-tert-butylphenyl}$), $\text{C}_{18}\text{H}_{29}\text{ITe}$, exhibits discrete molecules without $\text{Te}\cdots\text{I}$, $\text{Te}\cdots\text{Te}$ or $\text{I}\cdots\text{I}$ intermolecular contacts. The compound was prepared by cleavage of its parent ditellane with iodine, and represents a kinetically stabilized arenetellurenyl iodide with a very bulky substituent. The molecule possesses an angular $\text{C}-\text{Te}-\text{I}$ arrangement [$95.75(8)^\circ$] with a $\text{Te}-\text{I}$ single bond [$2.7181(6)\text{ \AA}$].

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Comment

Since the very unstable tellurenyl halides $R\text{TeHal}$ ($\text{Hal} = \text{Cl}, \text{Br}, \text{I}$) usually undergo rapid dismutation or disproportionation reactions, the stabilization of tellurenyl species in general can be attained by the use of either kinetic stabilization with bulky substituents or coordinating functional groups. In this fashion, $2,4,6\text{-}R_3\text{C}_6\text{H}_2\text{TeHal}$ [$R = \textit{i-Pr}$ (Trip), $\textit{i-Bu}$ (Mes^*); $\text{Hal} = \text{Br}, \text{I}$] (Du Mont *et al.*, 1992), TsiTeHal [$\text{Tsi} = \text{tris}(\text{trimethylsilyl})\text{methyl}$; $\text{Hal} = \text{Cl}, \text{Br}, \text{I}$] (Giselbrecht *et al.*, 1989), as well as several donor-stabilized tellurenyl halides, have been isolated (Sudha & Singh, 1994; Kaur *et al.*, 1995). To our knowledge, prior to our work, the only structurally characterized organotellurenyl (pseudo)halide species without additional functional groups was the tetrameric $(\text{PhTeI})_4$ (Schulz Lang *et al.*, 1999; Boyle *et al.*, 2000).



During the course of our investigations of organotellurenyl azides (Klapötke, Krumm, Nöth *et al.*, 2005), we were able to obtain the crystal structure of the benzenetellurenyl iodide Mes^*TeI , (I), and the alkanetellurenyl iodide TpsiTeI [Tpsi is $\text{tris}(\text{dimethylphenylsilyl})\text{methyl}$; Klapötke, Krumm & Schwab, 2005].

The crystal structure of (I) (Fig. 1) features a kinetically stabilized monomer; neither the Te nor the I atoms show intermolecular secondary interactions. For the benzene ring of (I), a strong deviation from planarity is observed [$\text{C}3-\text{C}2-\text{C}1-\text{C}6 = -9.2(5)^\circ$]. A comparable divergence has been reported for the homologous selenenyl compound, Mes^*SeI (Du Mont *et al.*, 1987).

A brief comparison of structural parameters for Mes^*TeI , (I), and the alkanetellurenyl derivative TpsiTeI can be found in the following communication (Klapötke, Krumm & Schwab, 2005).

Experimental

To a dark-red solution of 0.33 mmol bis(2,4,6-tri-*tert*-butylphenyl) ditellane (Mes*Te)₂ (Du Mont *et al.*, 1988) in 25 ml of toluene were added 0.33 mmol iodine in 10 ml of toluene. After stirring for 1 h at ambient temperature, the green solution was evaporated *in vacuo*. Recrystallization at 277 K from *n*-pentane yielded thin green needles of Mes*TeI after several days.

Crystal data

C ₁₈ H ₂₆ ITe	$D_x = 1.702 \text{ Mg m}^{-3}$
$M_r = 499.93$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5000 reflections
$a = 17.805 (4) \text{ \AA}$	$\theta = 2.3\text{--}25.9^\circ$
$b = 6.0230 (12) \text{ \AA}$	$\mu = 3.10 \text{ mm}^{-1}$
$c = 18.504 (4) \text{ \AA}$	$T = 200 (2) \text{ K}$
$\beta = 100.47 (3)^\circ$	Rod, green
$V = 1951.3 (7) \text{ \AA}^3$	$0.35 \times 0.08 \times 0.05 \text{ mm}$
$Z = 4$	

Data collection

Stoe IPDS diffractometer	3761 independent reflections
φ scans	3019 reflections with $I > 2\sigma(I)$
Absorption correction: numerical [<i>X-SHAPE</i> (Stoe & Cie, 1997) and <i>X-RED32</i> (Stoe & Cie, 1997)]	$R_{\text{int}} = 0.059$
$T_{\text{min}} = 0.543$, $T_{\text{max}} = 0.877$	$\theta_{\text{max}} = 25.9^\circ$
13085 measured reflections	$h = -21 \rightarrow 19$
	$k = -7 \rightarrow 7$
	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.026$	$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2]$
$wR(F^2) = 0.062$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.93$	$(\Delta/\sigma)_{\text{max}} = 0.001$
3761 reflections	$\Delta\rho_{\text{max}} = 0.65 \text{ e \AA}^{-3}$
190 parameters	$\Delta\rho_{\text{min}} = -1.18 \text{ e \AA}^{-3}$

Table 1

 Selected geometric parameters (\AA , $^\circ$).

I1—Te1	2.7181 (6)	Te1—C1	2.155 (3)
C1—Te1—I1	95.75 (8)	C6—C1—Te1	119.5 (2)
C2—C1—Te1	119.3 (2)		

H atoms were placed in geometrically idealized positions (C—H = 0.95 \AA and 0.98 \AA for aromatic CH and methyl groups, respectively) and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The methyl groups were allowed to rotate but not to tip. The highest residual electron density is located 1.02 \AA from I1 and the deepest hole is located 0.76 \AA from I1.

Data collection: *IPDS EXPOSE* (Stoe & Cie, 1996); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997);

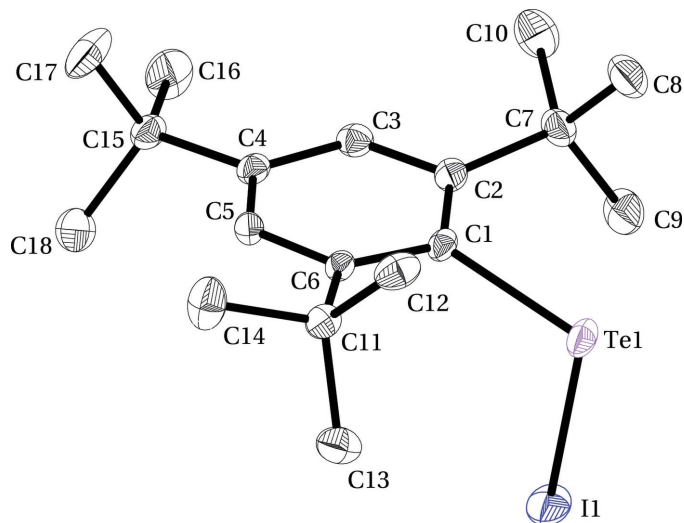


Figure 1

Drawing of the molecule of (I), with displacement ellipsoids at the 40% probability level. H atoms have been omitted.

molecular graphics: *DIAMOND* (Brandenburg, 1996); software used to prepare material for publication: *SHELXL97*.

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