Acta Crystallographica Section E Structure Reports Online

ISSN 1600-5368

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#### **Key indicators**

Single-crystal X-ray study T = 200 KMean  $\sigma(C-C) = 0.005 \text{ Å}$  R factor = 0.031 wR factor = 0.073 Data-to-parameter ratio = 22.5

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

# Tris(dimethylphenylsilyl)methanetellurenyl iodide

The crystal structure of TpsiTeI [Tpsi = tris(dimethylphenylsilyl)methyl],  $C_{25}H_{33}ISi_3Te$ , exhibits discrete molecules without Te···I, Te···Te or I···I intermolecular contacts. TpsiTeI was prepared by cleavage of its parent ditellane with iodine, and represents a kinetically stabilized alkanetellurenyl iodide with a very bulky substituent. The molecule possesses an angular C-Te-I arrangement [110.53 (7)°] with a Te-I single bond [2.7178 (7) Å]. Received 25 October 2005 Accepted 1 November 2005 Online 10 November 2005

# Comment

During the course of our investigations of organotellurenyl azides (Klapötke, Krumm, Nöth *et al.*, 2005), we were able to determine the crystal structure of the benzenetellurenyl iodide Mes\*TeI (Klapötke, Krumm & Schwab, 2005) and the alkanetellurenyl derivative TpsiTeI, (I) (Fig. 1).



As can be seen, the crystal structures of both compounds feature kinetically stabilized monomers; neither the Te nor the I atoms show intermolecular secondary interactions.

The Te-I bonds in (I) and Mes\*TeI (Klapötke, Krumm & Schwab, 2005) are very similar [2.7178 (7) versus 2.7181 (6) Å]; however, a large difference is found in the C-Te-I angles [110.53 (7) versus 95.75 (8)°]. This can be attributed to the increased bulkiness of the trisilylmethyl compared to the 2,4,6-tri-*tert*-butylphenyl substituent. In between these two, the steric influence of the terphenyl derivative 2,6-Trip<sub>2</sub>C<sub>6</sub>H<sub>3</sub>TeI [Te-I = 2.617 (1) Å and C-Te-I = 106.2 (2)°] can be estimated (Klapötke, Krumm, Nöth *et al.* 2005).

# **Experimental**

To a green solution of 0.28 mmol bis[tris(phenyldimethylsilyl)methyl] ditellane (TpsiTe)<sub>2</sub> (Klapötke, Krumm, Nöth *et al.* 2005) in 10 ml of benzene were added 0.23 mmol of neat iodine. After stirring for 1 h at ambient temperature, the dark-blue–green solution was evaporated *in vacuo*. Recrystallization at 277 K from n-pentane yielded dark-green blocks of TpsiTeI after several days.

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# organic papers

### Crystal data

C25H33ISi3Te
$M_r = 672.28$
Monoclinic, $P2_1/c$
a = 16.076 (3) Å
b = 17.248 (3)Å
c = 9.995 (2) Å
$\beta = 101.18 \ (3)^{\circ}$
$V = 2718.9 (9) \text{ Å}^3$
Z = 4

#### Data collection

Nonius KappaCCD diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: none
12153 measured reflections
6229 independent reflections
4995 reflections with $I > 2\sigma(I)$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_0^2) + (0.0278P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.031$	+ 1.9905P]
$wR(F^2) = 0.073$	where $P = (F_0^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{\rm max} = 0.002$
6229 reflections	$\Delta \rho_{\rm max} = 0.79 \ {\rm e} \ {\rm \AA}^{-3}$
277 parameters	$\Delta \rho_{\rm min} = -1.35 \text{ e } \text{\AA}^{-3}$
H-atom parameters constrained	

 $D_x = 1.642 \text{ Mg m}^{-3}$ 

Cell parameters from 6375 reflections  $\theta = 3.1-27.5^{\circ}$ 

Mo  $K\alpha$  radiation

 $\mu = 2.37 \text{ mm}^{-1}$ 

T = 200 (2) K

 $R_{\rm int} = 0.023$ 

 $\theta_{\rm max} = 27.5^{\circ}$  $h = -20 \rightarrow 20$ 

 $k = -22 \rightarrow 21$ 

 $l = -12 \rightarrow 12$ 

Block, dark green  $0.08 \times 0.05 \times 0.04 \text{ mm}$ 

#### Table 1

Selected geometric parameters (Å, °).

I1-Te1	2.7178 (7)	Si2-C10	1.870 (3)
Te1-C1	2.212 (3)	Si2-C12	1.888 (3)
Si1-C2	1.869 (3)	Si2-C1	1.917 (3)
Si1-C3	1.870 (3)	Si3-C18	1.866 (3)
Si1-C4	1.898 (3)	Si3-C19	1.880 (3)
Si1-C1	1.942 (3)	Si3-C20	1.892 (3)
Si2-C11	1.865 (3)	Si3-C1	1.925 (3)
C1-Te1-I1	110.53 (7)		

H atoms were placed in geometrically idealized positions (C–H = 0.95 Å and 0.98 Å for aromatic CH and methyl groups, respectively) and constrained to ride on their parent atoms, with  $U_{iso}(H) = 1.2U_{eq}(C)$ . The methyl groups were allowed to rotate but not to tip. The highest residual electron density is located 0.96 Å from Te1 and the deepest hole is located 0.75 Å from I1.

Data collection: *COLLECT* (Nonius, 2000); 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); molecular graphics: *DIAMOND* (Brandenburg, 1996); software used to prepare material for publication: *SHELXL97*.



#### Figure 1

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

The authors thank Dr P. Mayer for data collection and the Ludwig–Maximilian University for financial support of this work.

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