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Bis(1-naphthyl) ditelluride

**Ernesto Schulz Lang,* Robert Alan Burrow and
Edson Tarabal Silveira**

Departamento de Química, Universidade Federal de Santa Maria, Santa Maria, RS,
97119-900, Brazil
Correspondence e-mail: eslang@quimica.ufsm.br

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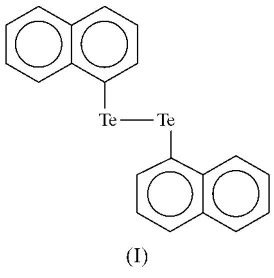
The title compound, $C_{20}H_{14}Te_2$, shows a *transoid* conformation, with a C—Te—Te—C torsion angle of 97.96 (9)°. The Te—Te units show approximate η^6 interactions with neighbouring naphthyl groups, forming chains along the *c* axis. The molecule lies about a crystallographic twofold axis.

Comment

We have found the diorganoditelluride compounds *R*Te—Te*R* to be optimal synthons for the synthesis of new organotellurium metal complexes or clusters (Schulz Lang *et al.*, 1994; Schulz Lang, Gatto & Abram, 2002; Schulz Lang, Zan *et al.*, 2002). The naphthyl moiety gives rise to various conformational forms with different cell packing, leading to different steric and electronic effects (Sandman *et al.*, 1994; Engman & Cava, 1982; Menon *et al.*, 1996). In this paper, we report the preparation and structural characterization of, and some observations on, the title compound, (I).



(I)

Single crystals of (I) were obtained by slow evaporation of a solution in tetrahydrofuran, in the presence of air, of the crude product from the reaction of 1-naphthylmagnesium bromide and tellurium in tetrahydrofuran. The asymmetric unit of (I) contains half a molecule of the ditelluride. The complete molecule is generated by the operation on the half molecule of a twofold axis parallel to *c*. Selected bond distances and angles are given in Table 1.

The Te—Te bond length in (I) of 2.7110 (6) Å is close to that found for the two conformational polymorphs of bis(2-naphthyl) ditelluride, 2.7089 (7) and 2.7179 (6) Å (Sandman *et al.*, 1994). The Te—Te—C angle of 97.96 (9)° is within the range found for substituted diphenyl ditellurides (92.9–101.7°; Schulz Lang *et al.*, 1994). The C—Te—Te—C torsion angle for (I) is 97.96 (9)° and this may be considered a *transoid* conformation (C—Te—Te—C > 90°). The two polymorphs of bis(2-naphthyl) ditelluride have torsion angles of 105.2 (3)° for the *trans* and 78.6 (2)° for the *cis* form.

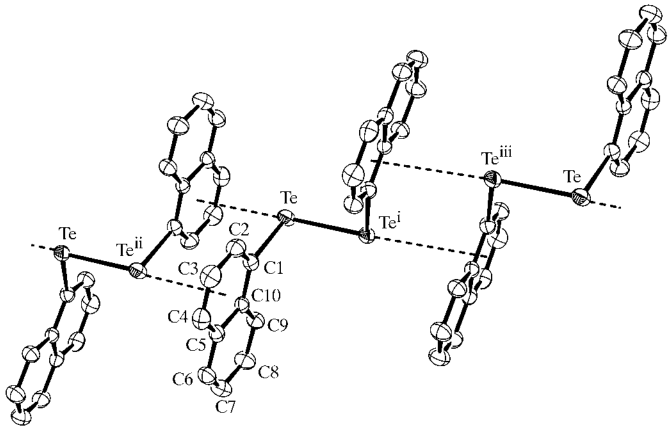


Figure 1
A view of the molecule of (I) with the atomic labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity. The dashed lines indicate η^6 interactions. [Symmetry codes: (i) $-x, y, \frac{1}{2} - z$; (ii) $-x, 2 - y, -z$; (iii) $x, 2 - y, \frac{1}{2} + z$.]

The ditelluride unit is capped on either end by approximate η^6 interactions to neighbouring naphthyl groups (Fig. 1). The Te—Te vector is closer to atoms C5 and C10, indicating that the ring interaction is slipped slightly towards the middle of the naphthyl group. The distance from the Te atom to the centroid, *Cg*, of the C_6 ring (C1–C5/C10) bonded to the neighbouring Te atom is 3.683 (2) Å, with a Te—Te—*Cg* angle of 162.46 (2)°. This forms continuous chains along the *c* axis. Similar interactions have been found for the *transoid* form of bis(2-naphthyl) ditelluride and diphenyl ditelluride (Llabres *et al.*, 1972), with Te—*Cg* distances of 3.620 and 3.601 Å, respectively.

Another interesting example has been observed with bis[8-(dimethylamino)-1-naphthyl] ditelluride (Menon *et al.*, 1996), where the Te—Te bond [2.765 (1) Å] is slightly longer than in (I) and the other examples mentioned above. The longer Te—Te distance in this case is presumably due to a strong Te···N interaction.

Experimental

To a solution of 1-naphthylmagnesium bromide, prepared from 1-bromonaphthalene (16.71 ml, 78.36 mmol) and Mg (1.93 g, 78.36 mmol) in tetrahydrofuran (250 ml), was added Te shot (10.0 g, 78.36 mmol) at room temperature. The Te mixture was stirred under reflux for 3 h and then cooled to 273 K and treated with a saturated solution of NH_4Cl (60 ml, vigorous evolution of gas). The mixture was filtered and the solids washed with a saturated aqueous solution of NH_4Cl and ether. The organic phase was dried with Na_2SO_4. Evaporation of the solvent and recrystallization from $CHCl_3$ and petroleum ether afforded pure (I).

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Crystal data

$C_{20}H_{14}Te_2$
$M_r = 509.52$
Monoclinic, $C2/c$
$a = 16.675\ (3)$ Å
$b = 7.8710\ (14)$ Å
$c = 14.339\ (3)$ Å
$\beta = 116.839\ (3)^\circ$
$V = 1679.2\ (5)$ Å^3
$Z = 4$

$D_x = 2.015$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2734 reflections
$\theta = 5.5$–54.7°
$\mu = 3.47$ mm^{-1}
$T = 293\ (2)$ K
Block, red
0.22 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD1000 area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.537$, $T_{\max} = 0.707$
5118 measured reflections

1952 independent reflections
1648 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.032$
$\theta_{\max} = 28^\circ$
$h = -19 \rightarrow 22$
$k = -10 \rightarrow 10$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.069$
$S = 0.97$
1952 reflections
128 parameters

All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 1.30$ e Å^{-3}
$\Delta\rho_{\min} = -0.49$ e Å^{-3}

Table 1

Selected geometric parameters (Å, °).

Te—C1	2.135 (3)	Te—Te$^{\rm i}$	2.7110 (6)
C1—Te—Te$^{\rm i}$	97.96 (9)		

Symmetry code: (i) $-x, y, \frac{1}{2} - z$.

The largest peak in the difference map was 0.82 Å from Te and the deepest hole was 0.74 Å from Te.

Data collection: *SMART* (Bruker, 1997); cell refinement: Bruker software *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: TA1375). Services for accessing these data are described at the back of the journal.

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