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Dibromobis(4-methoxyphenyl)tellurium(IV)

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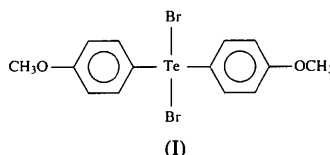
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Abstract

The structure analysis shows that the title compound, $[\text{TeBr}_2(\text{C}_7\text{H}_7\text{O})_2]$, is isostructural with the corresponding dichloro compound. There are two molecules in the asymmetric unit in which the Te atom has pseudo-trigonal bipyramidal coordination geometry. The two independent molecules, along with their centrosymmetric equivalents, form isolated tetramers by means of $\text{Te} \cdots \text{Br}$ contacts ranging from 3.535 (1) to 3.741 (1) Å.

Comment

As a continuation of our spectroscopic and structural work in the field of organotellurium compounds (Torres, 1990; de Matheus, Torres, Piniella, Briansó & Miravittles, 1991; Farran, Alvarez-Larena, Piniella, Germain & Torres, 1994), we have determined the structure of the title compound, (I).



The structure found for the title compound confirms the results of previous spectroscopic studies: ^1H NMR (Berry, Kustan, Roshani & Smith, 1975; Ley, Meerholz & Barton, 1981), ^{13}C NMR (Chadha & Miller, 1982), low-frequency IR (McWhinnie & Patel, 1972) and ^{125}Te Mössbauer (Berry & Jones, 1976).

The two independent molecules present in the asymmetric unit have similar conformations, differing mainly

in the orientation of one methoxy group ($\text{O3}-\text{C37}$). The phenyl rings are in a propeller arrangement. The intramolecular geometry around the Te atoms is pseudo-trigonal bipyramidal, with Br atoms in the apical positions and the Te lone pair occupying the fifth position in the equatorial plane, as expected for a non-ionic $R_2\text{TeX}_2$ compound (Mangion, Zingaro & Meyers, 1975). Dibromobis(4-methoxyphenyl)tellurium displays the longest and the shortest Te—Br bond lengths when compared with the other known structures having a $\text{C}_2-\text{Te}-\text{Br}_2$ subunit (Christofferson & McCullough, 1958; Chadha & Nguyen, 1990; Knobler & McCullough, 1972; Detty & Luss, 1986). The length of the Te—Br bond depends on the intermolecular contacts. Three situations are found: firstly, when the Br atoms do not participate in any interaction the distance is the shortest [Te_2-Br_3 2.629 (1) Å]; second, when a Br atom is involved in one intermolecular contact with another Te atom, the distances are intermediate [Te_1-Br_1 and Te_1-Br_2 2.672 (1) and 2.677 (1) Å, respectively]; and third, when a Br atom forms two $\text{Te} \cdots \text{Br}$ contacts, the Te—Br distance is the longest [Te_2-Br_4 2.733 (1) Å]. The Te—C distances [2.110 (4)–2.116 (4) Å] are at the lower end of the range observed for the aforementioned dibromo compounds. Another interesting feature is that the Br—Te—Br angles [179.12 (2) and 179.44 (2)°] are closer to the ideal value of 180° than in the other structures.

Taking into account the intermolecular contacts, the coordination around the Te atoms may be considered to be octahedral. The title compound is isostructural with the dichloro analogue [$\text{TeCl}_2(\text{C}_7\text{H}_7\text{O})_2$] (Chadha & Drake, 1984). The packing consists of isolated tetramers formed by the two molecules of the asymmetric unit and the two generated by a centre of symmetry. The four molecules are connected through $\text{Te} \cdots \text{Br}$ contacts. This pattern is similar to that seen for [$\text{TeCl}_2(\text{C}_6\text{H}_5)(p\text{-BrC}_6\text{H}_4)$] (Chadha, Drake & Khan, 1983) and [$\text{TeCl}_2(\text{C}_{12}\text{H}_8\text{O})$] (Korp, Bernal, Turley & Martin, 1980).

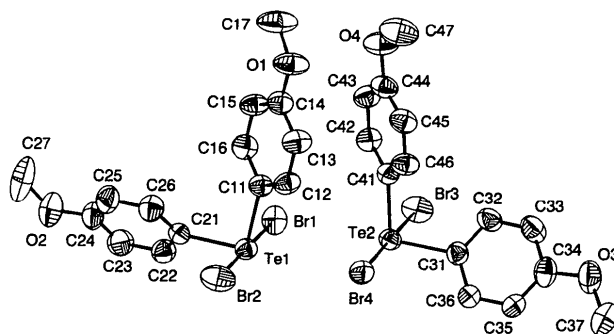


Fig. 1. Drawing of dibromobis(4-methoxyphenyl)tellurium showing the two molecules of the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level.

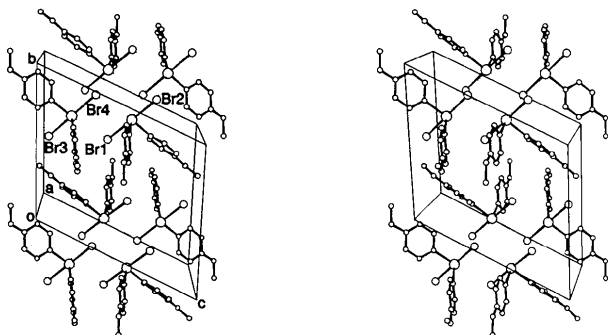


Fig. 2. Stereoview of the unit-cell packing showing the tetramers.

Experimental

The compound was synthesized according to the method of Lederer (1916) and suitable crystals were grown by slow evaporation from an acetone solution.

Crystal data

[TeBr₂(C₇H₇O)₂]

$M_r = 501.67$

Triclinic

$P\bar{1}$

$a = 10.319 (1) \text{ \AA}$

$b = 12.716 (1) \text{ \AA}$

$c = 13.9132 (7) \text{ \AA}$

$\alpha = 109.841 (5)^\circ$

$\beta = 100.207 (6)^\circ$

$\gamma = 101.960 (8)^\circ$

$V = 1618.1 (2) \text{ \AA}^3$

$Z = 4$

$D_x = 2.059 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71069 \text{ \AA}$

Cell parameters from 25

reflections

$\theta = 11.39\text{--}13.88^\circ$

$\mu = 6.77 \text{ mm}^{-1}$

$T = 293 (2) \text{ K}$

Prism

$0.44 \times 0.26 \times 0.11 \text{ mm}$

Bright yellow

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
Te1	0.37999 (3)	0.89048 (2)	0.57682 (2)	0.0426 (1)
Br1	0.38623 (6)	0.69102 (5)	0.43208 (4)	0.0612 (2)
Br2	0.37469 (6)	1.09145 (5)	0.72072 (5)	0.0756 (2)
C11	0.1702 (4)	0.8169 (4)	0.5603 (3)	0.044 (1)
C12	0.0763 (5)	0.8767 (4)	0.5414 (4)	0.051 (1)
C13	-0.0603 (5)	0.8289 (4)	0.5303 (4)	0.057 (1)
C14	-0.1041 (5)	0.7234 (4)	0.5394 (4)	0.053 (1)
C15	-0.0113 (5)	0.6635 (4)	0.5580 (4)	0.053 (1)
C16	0.1269 (5)	0.7117 (4)	0.5682 (4)	0.054 (1)
O1	-0.2407 (3)	0.6858 (3)	0.5296 (3)	0.074 (1)
C17	-0.2940 (6)	0.5732 (5)	0.5314 (6)	0.097 (2)
C21	0.4586 (4)	0.8368 (4)	0.6975 (3)	0.043 (1)
C22	0.5757 (5)	0.8022 (4)	0.6955 (4)	0.053 (1)
C23	0.6312 (5)	0.7681 (5)	0.7725 (4)	0.064 (1)
C24	0.5671 (6)	0.7685 (5)	0.8525 (4)	0.064 (1)
C25	0.4524 (6)	0.8034 (5)	0.8558 (4)	0.067 (1)
C26	0.3969 (5)	0.8398 (5)	0.7785 (4)	0.060 (1)
O2	0.6318 (5)	0.7304 (4)	0.9236 (3)	0.091 (1)
C27	0.5663 (8)	0.7144 (7)	0.9994 (5)	0.127 (3)
Te2	0.25312 (3)	0.74457 (2)	0.20666 (2)	0.0434 (1)
Br3	0.25494 (6)	0.54530 (5)	0.06625 (5)	0.0700 (2)
Br4	0.25551 (5)	0.95303 (4)	0.35325 (4)	0.0550 (1)
C31	0.1720 (5)	0.7946 (4)	0.0839 (3)	0.046 (1)
C32	0.0539 (5)	0.7209 (4)	0.0054 (4)	0.057 (1)
C33	0.0019 (6)	0.7543 (4)	-0.0744 (4)	0.064 (1)
C34	0.0677 (6)	0.8575 (5)	-0.0784 (4)	0.060 (1)
C35	0.1864 (5)	0.9304 (4)	-0.0017 (4)	0.059 (1)
C36	0.2384 (5)	0.8984 (4)	0.0804 (4)	0.057 (1)
O3	0.0064 (4)	0.8799 (3)	-0.1619 (3)	0.079 (1)
C37	0.0606 (7)	0.9908 (5)	-0.1660 (4)	0.080 (2)
C41	0.0621 (4)	0.6646 (4)	0.2234 (4)	0.046 (1)
C42	0.0415 (5)	0.5601 (4)	0.2339 (4)	0.050 (1)
C43	-0.0827 (5)	0.5083 (4)	0.2464 (4)	0.058 (1)
C44	-0.1867 (5)	0.5614 (4)	0.2486 (4)	0.054 (1)
C45	-0.1646 (5)	0.6673 (4)	0.2385 (4)	0.057 (1)
C46	-0.0407 (5)	0.7185 (4)	0.2260 (4)	0.054 (1)
O4	-0.3044 (4)	0.5036 (3)	0.2604 (3)	0.075 (1)
C47	-0.4155 (6)	0.5544 (6)	0.2615 (6)	0.096 (2)

Table 2. Selected geometric parameters (\AA , $^\circ$)

Te1—C11	2.110 (4)	Te2—C41	2.114 (4)
Te1—C21	2.114 (4)	Te2—C31	2.116 (4)
Te1—Br1	2.672 (1)	Te2—Br3	2.629 (1)
Te1—Br2	2.677 (1)	Te2—Br4	2.733 (1)
Te1...Br4 ⁱ	3.652 (1)	Te2...Br2 ⁱ	3.741 (1)
Te1...Br4	3.556 (1)	Te2...Br1	3.535 (1)
C11—Te1—C21	96.4 (2)	C21—Te1—Br4 ⁱ	79.9 (1)
C11—Te1—Br1	90.4 (1)	Br1—Te1—Br4	84.44 (2)
C21—Te1—Br1	89.1 (1)	Br1—Te1—Br4 ⁱ	97.57 (2)
C11—Te1—Br2	90.0 (1)	Br2—Te1—Br4	95.14 (2)
C21—Te1—Br2	91.3 (1)	Br2—Te1—Br4 ⁱ	82.14 (2)
Br1—Te1—Br2	179.44 (2)	Br4—Te1—Br4 ⁱ	99.90 (2)
C41—Te2—C31	96.6 (2)	C31—Te2—Br1	173.5 (1)
C41—Te2—Br3	91.1 (1)	C31—Te2—Br2 ⁱ	100.6 (1)
C31—Te2—Br3	90.7 (1)	C41—Te2—Br1	83.1 (1)
C41—Te2—Br4	89.7 (1)	C41—Te2—Br2 ⁱ	159.7 (1)
C31—Te2—Br4	89.5 (1)	Br3—Te2—Br1	95.81 (2)
Br3—Te2—Br4	179.12 (2)	Br3—Te2—Br2 ⁱ	99.36 (2)
C11—Te1—Br4	84.8 (1)	Br4—Te2—Br1	83.98 (2)
C11—Te1—Br4 ⁱ	171.1 (1)	Br4—Te2—Br2 ⁱ	79.76 (2)
C21—Te1—Br4	173.5 (1)	Br1—Te2—Br2 ⁱ	78.63 (2)

Symmetry code: (i) $1 - x, 2 - y, 1 - z$.

Data collection

Enraf-Nonius CAD-4 diffractometer

$\omega/2\theta$ scans

Absorption correction:

empirical (North, Phillips & Mathews, 1968)

$T_{\min} = 0.4442$, $T_{\max} = 0.9998$

5675 measured reflections

5675 independent reflections

3672 observed reflections

$[I > 2\sigma(I)]$

$\theta_{\max} = 24.97^\circ$

$h = -12 \rightarrow 11$

$k = -15 \rightarrow 14$

$l = 0 \rightarrow 16$

3 standard reflections

frequency: 120 min

intensity decay: none

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.0311$

$wR(F^2) = 0.0776$

$S = 1.229$

5675 reflections

345 parameters

Only H-atom U 's refined

$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = -0.188$

$\Delta\rho_{\max} = 0.343 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -1.069 \text{ e \AA}^{-3}$

Extinction correction: none

Atomic scattering factors

from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Data collection and cell refinement: CAD-4 diffractometer software. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure:

SHELXL93 (Sheldrick, 1993). Molecular graphics: *PC-ORTEP* (Schmid & Brueggemann, 1990a), *PC-PLUTO* (Schmid & Brueggemann, 1990b).

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Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: NA1109). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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