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(2-Phenylethyl)ammonium tetrabromothallate(III)

M. Abdi,[a]* F. Zouari,[a] N. Chniba-Boudjada,[b] P. Bordet[b] and A. Ben Salah[a]

[a]Laboratoire de Sciences des Materiaux et d'Environnement, Faculte des Sciences de Sfax, Tunisia, and [b]Laboratoire de Cristallographie CNRS, BP166, 38042 Grenoble Cedex 9, France

Correspondence e-mail: abdi_monia@yahoo.fr

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.029 Å
R factor = 0.051
wR factor = 0.132
Data-to-parameter ratio = 24.9

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

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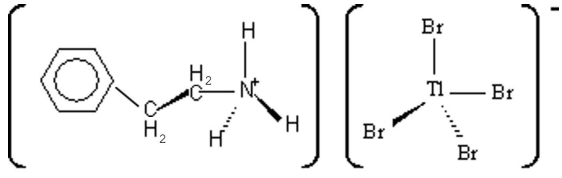
The structure of the title compound, $(C_8H_{12}N)[TlBr_4]$, is characterized by tetracoordinate thallium, forming a regular tetrahedron $TlBr_4$ with Tl—Br distances ranging between 2.528 (2) and 2.562 (2) Å. Chains of $TlBr_4$ tetrahedra oriented along the c axis form pseudo-hexagonal rings, containing two columns formed by obliquely stacked amine cations.

Comment

The title compound, (I), belongs to the system of general formula $LTlX_4$ (where L is an organic cation and X is Br) which form part of the compound type L_nTlX_m [where L is a neutral organic ligand or organic cation, X = Br, Cl or I, and m = 3, 4 or 5 (Bermejo *et al.*, 1991; James *et al.*, 1996; Linden *et al.*, 2003)]. Structural phase transitions and interesting physical properties have been observed and reported for these compounds (Walton, 1968; Abdi, Zouari, Chaabouni *et al.*, 2003; Abdi, Zouari, Chaabouni & Ben Salah, 2003). The Tl atom can be coordinated by four, five or six neighbours, leading to a variety of geometrical arrangements, such as tetrahedral, square pyramidal or trigonal bipyramidal, and octahedral (Linden *et al.*, 1999, 2003; Abdi *et al.*, 2004). As part of our interest in the environment of Tl in bromo complexes, we report here the structure determination of a new halo-compound, (2-phenylethyl)ammonium tetrabromothallate(III), (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The asymmetric unit contains one (2-phenylethyl)ammonium cation and one $TlBr_4^-$ anion; the latter is arranged as an almost regular tetrahedron, with Tl—Br distances ranging from 2.528 (2) to 2.562 (2) Å. The structural arrangement, shown in Fig. 2, is strongly one-dimensional. Tetrahedral $TlBr_4^-$ anions form chains along the c axis. These chains are related by the 2_1 axis and form elongated pseudo-hexagonal rings which contain two columns of the amine cations. The planar benzene rings make an angle of approximately 45° with the c axis. Due to the elongation of the pseudo-hexagonal rings, one can also consider alternating layers of the amine cations and $TlBr_4^-$ anions being stacked along the a axis.

Experimental

Yellow–orange crystals of (I) were obtained by slow evaporation of a solution of thallium(III) oxide and 2-phenylethylamine in concentrated HBr. The reaction occurs in the presence of ethanol (50 ml) and acetone (20 ml).

Crystal data

$(C_8H_{12}N)[TlBr_4]$
M_r = 646.18
Orthorhombic, $Pna2_1$
a = 17.944 (1) Å
b = 11.9692 (6) Å
c = 6.9072 (3) Å
V = 1483.50 (13) Å^3
Z = 4
D_x = 2.895 Mg m^{-3}
Ag $K\alpha$ radiation
Cell parameters from 1924 reflections
θ = 3.1–18.4°
μ = 11.71 mm^{-1}
T = 298 K
Parallelepiped, yellow–orange
0.52 × 0.13 × 0.12 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: by Gaussian integration (Coppens, 1970)
T_{min} = 0.139, T_{max} = 0.288
6988 measured reflections
3190 independent reflections
2167 reflections with $I > 2\sigma(I)$
R_{int} = 0.082
θ_{max} = 21.4°
$h = -23 \rightarrow 23$
$k = -12 \rightarrow 15$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.132
S = 1.03
3190 reflections
128 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.52 e Å^{-3}
$\Delta\rho_{min}$ = −1.67 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0081 (6)
Absolute structure: Flack (1983), 1348 Friedel pairs
Flack parameter = 0.02 (4)

Table 1
Selected geometric parameters (Å, °).

Br2—Tl	2.545 (2)	Br4—Tl	2.562 (2)
Br3—Tl	2.528 (2)	Br1—Tl	2.545 (2)
Br3—Tl—Br2	111.52 (8)	Br3—Tl—Br4	105.68 (8)
Br3—Tl—Br1	112.17 (8)	Br2—Tl—Br4	110.76 (7)
Br2—Tl—Br1	109.12 (8)	Br1—Tl—Br4	107.49 (8)

The H atoms were positioned geometrically and refined as riding, with C—H = N—H = 0.96 Å and $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DIRAX/LSQ* (Duisenberg & Schreurs, 2000); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

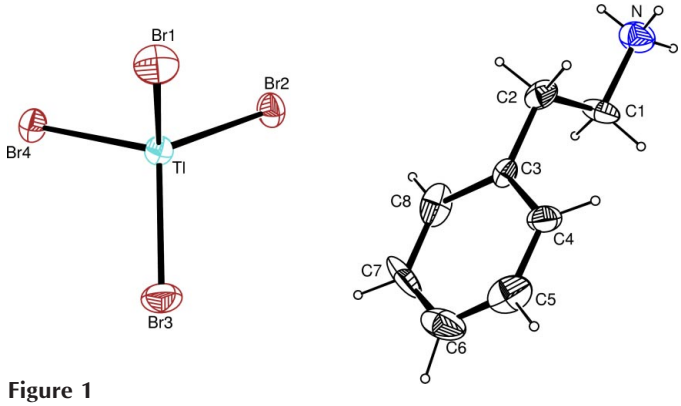


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids.

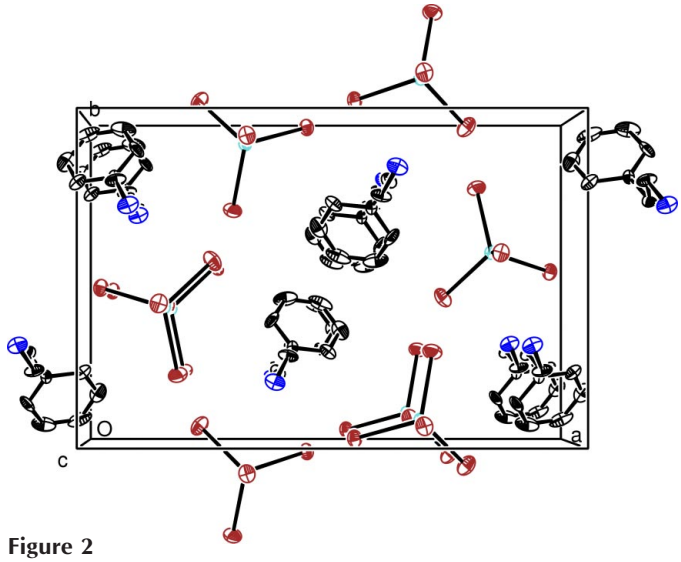


Figure 2
Perspective view along the c axis, showing pseudo-hexagonal rings of chains of $TlBr_4^-$ anions. H atoms have been omitted.

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