Refinement of the crystal structure of dithallium(I) trioxotellurate(IV), Tl_2TeO_3

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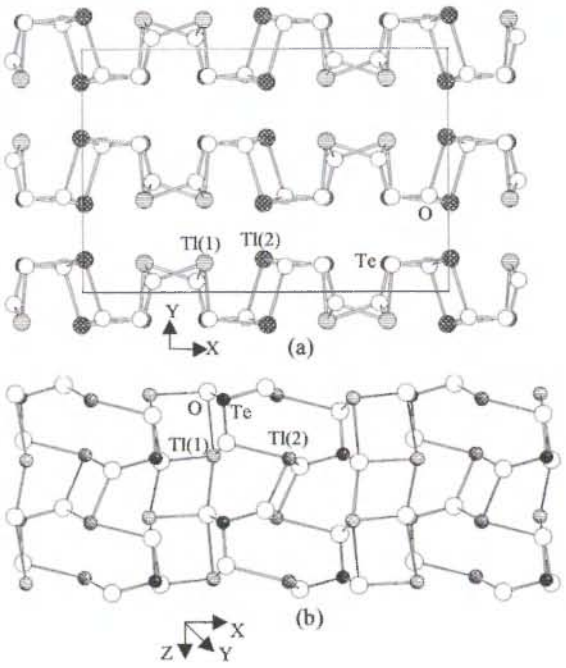

Abstract

O_3TeTl_2, orthorhombic, *Pban* (No. 50), $a = 16.60(1)$ Å, $b = 11.078(6)$ Å, $c = 5.238(1)$ Å, $V = 963.2$ Å^3, $Z = 8$, $R_{gt}(F) = 0.047$, $wR(F^2) = 0.090$, $T = 293$ K.

Source of material

Single crystals of Tl_2TeO_3 were obtained by heating the Tl_2TeO_3 crystalline compound in a gold crucible at 673 K for 12 hours under pure flowing nitrogen and then cooling (3K/h) it down to 173 K.

Discussion

In the original crystal structure of Tl_2TeO_3 [1], the Te(IV) atoms were irregularly coordinated to three oxygen atoms (Te–O distances: 1.826 Å, 1.828 Å and 1.891 Å) at the centre of a distorted TeO_3E tetrahedron whose one corner was occupied by the stereochemically active lone pair $5s^2$ of this atom. Two of these bond lengths (1.826 Å and 1.828 Å) were abnormally short (less than the Te–O distance observed in the gaseous TeO_2 molecule [2]), leading to a bond valence sum a bit too high (4.23) [3, 4]. In the refined structure a more regular TeO_3E polyhedron is observed with nearly three identical Te–O bond lenghts (1.868(8) Å; 1.871(10) Å and 1.877(9) Å; bond valence sum: 3.98). The crystal structure of Tl_2TeO_3 is of distorted NaCl type. The strong stereochemical activity of the lone pairs E of Te and Tl atoms divides the structure into two-dimensional layers parallel to the (010) plane and constituted of $Tl(2)O_3E$, TeO_3E tetrahedra and $Tl(1)O_4E$ trigonal bipyramids sharing either edges or corners.

Table 1. Data collection and handling.

Crystal:	orange prism, size 0.03 × 0.12 × 0.30 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	726.36 cm^{-1}
Diffractometer, scan mode:	Siemens P4, ω
$2\theta_{max}$:	60.06°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1750, 1275
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 602
$N(param)_{refined}$:	56
Programs:	SHELXL-93 [5], SCHAKAL97 [6]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Tl(1)	8*m*	0.33198(3)	0.12048(5)	0.7526(1)	0.0305(3)	0.0196(3)	0.0277(3)	–0.0070(2)	–0.0007(5)	–0.0012(6)
Tl(2)	8*m*	0.49543(3)	0.13553(6)	0.2414(1)	0.0241(3)	0.0243(4)	0.0275(3)	0.0012(2)	–0.0026(5)	0.0028(5)
Te	8*m*	0.66358(5)	0.11395(9)	0.7629(2)	0.0210(4)	0.0149(4)	0.0196(4)	0.0004(3)	–0.0001(7)	–0.0003(8)
O(1)	8*m*	0.3114(5)	0.0503(9)	0.276(2)	0.027(4)	0.014(5)	0.038(6)	0.004(4)	–0.002(5)	–0.006(7)
O(2)	8*m*	0.4462(5)	0.895(1)	0.313(2)	0.017(4)	0.048(8)	0.022(5)	0.001(4)	0.001(4)	0.007(6)
O(3)	8*m*	0.3445(5)	0.889(1)	0.881(2)	0.029(5)	0.030(7)	0.027(5)	0.005(5)	–0.003(4)	–0.012(6)

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