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Crystal structure of bis(benzyltriethylammonium) hexachlorotellurate(IV), $[C_7H_7(C_2H_5)_3N]_2(TeCl_6)$

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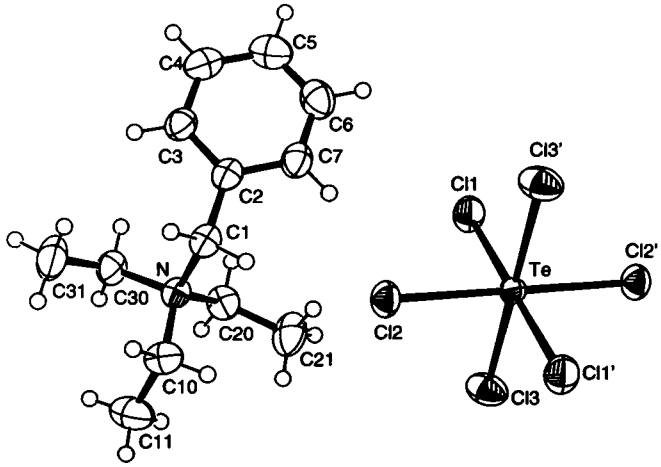

Abstract

$C_{26}H_{44}Cl_6N_2Te$, monoclinic, $P12_1/n1$ (no. 14),
$a = 9.3981(5)$ Å, $b = 14.606(1)$ Å, $c = 12.4524(7)$ Å,
$\beta = 108.335(5)°$, $V = 1622.6$ Å^3, $Z = 2$,
$R_{gt}(F) = 0.024$, $wR_{ref}(F^2) = 0.065$, $T = 293$ K.

Source of material

Tellurium tetrachloride and benzyltriethylammonium chloride, in dichlormethane, were mixed in a 1:2 molar ratio, yielding a yellow precipitate. After filtration, the yellow filtrate was allowed to stand at room temperature to dryness. Crystals were obtained by slow evaporation from CH_2Cl_2.

Discussion

The lattice consists of discrete $[TeCl_6]^{2-}$ anions and $[C_{13}H_{22}N]^+$ cations. The $[TeCl_6]^{2-}$ dianion resides on a centre of symmetry having an almost regular octahedral coordination. The Te—Cl2 distance (2.5457(5) Å) is longer than the other two, the Cl atom being involved in three short contacts: Cl2···H1b (2.93 Å, ∠Cl···H–C = 169.0°), Cl2···H11b^{i} (2.89 Å, 152.9°; i: $-x-½, y+½, -z+½$) and Cl2···H30b^{ii} (2.81 Å, 150.1°; ii: $x+½, -y+½, z+½$); the shortest corresponds to Te—Cl1 (2.5308(5) Å), the Cl1 atom is also involved in three short contacts: Cl1···H7 (2.86 Å, 136.6°), Cl1···H11c^{iii} (2.84 Å, 168.1°; iii: $-x+½, y+½, -z+½$) and Cl1···H20b^{iii} (2.92 Å, 141.4°). Cl3 which does not make any short contact has the medium Te—Cl distance (2.5404(6) Å). So that, whether or not these short contacts are hydrogen bonds is difficult to ascertain because, as pointed out by Cotton et al. [1], "the field is getting muddier and muddier as the definition of a hydrogen bond is relaxed". In any case, the Cl···H distances are shorter than the sum of the van der Waals radii of H and Cl (3.0 Å [2]). The $[TeCl_6]^{2-}$ bond angles are near 90° ranging from 88.09(2)° to 91.91(2)°.

The same trend in Te—Cl bond lengths has been found for the phenyltrimethylammonium salt [3], where the longest and the shortest distances correspond to chlorine atoms involved in three short Cl···H contacts and the medium corresponds to the one Cl atom involved only in one such contact.

Table 1. Data collection and handling.

Crystal:	yellow, irregular, size 0.15 × 0.20 × 0.25 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	14.29 cm^{-1}
Diffractometer, scan mode:	Enraf-Nonius CAD4, θ-2θ
$2\theta_{max}$:	59.94°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4971, 4714
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3754
$N(param)_{refined}$:	163
Programs:	SIR92 [4], SHELXL-97 [5], ZORTEP [6], PARST95 [7]

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

Atom	Site	x	y	z	U_{iso}
H(1A)	4e	−0.0384	0.1109	0.5015	0.044
H(1B)	4e	−0.0124	0.1146	0.3837	0.044
H(3)	4e	0.1933	0.0670	0.6740	0.055
H(4)	4e	0.3801	−0.0423	0.7303	0.064
H(5)	4e	0.4596	−0.1182	0.5979	0.070
H(6)	4e	0.3548	−0.0846	0.4083	0.068
H(7)	4e	0.1759	0.0279	0.3506	0.055
H(10A)	4e	−0.1068	0.2623	0.3428	0.056
H(10B)	4e	−0.1508	0.2560	0.4538	0.056
H(11A)	4e	−0.0383	0.3973	0.5124	0.095
H(11B)	4e	−0.1609	0.4071	0.3938	0.095
H(11C)	4e	0.0091	0.4034	0.4026	0.095
H(20A)	4e	0.2809	0.2161	0.4671	0.052
H(20B)	4e	0.2221	0.3170	0.4519	0.052
H(21A)	4e	0.1227	0.1826	0.2825	0.098
H(21B)	4e	0.2410	0.2581	0.2818	0.098
H(21C)	4e	0.0749	0.2859	0.2677	0.098
H(30A)	4e	0.2162	0.2156	0.6406	0.054
H(30B)	4e	0.1577	0.3158	0.6121	0.054
H(31A)	4e	−0.0670	0.2776	0.6403	0.099
H(31B)	4e	0.0655	0.2509	0.7484	0.099
H(31C)	4e	−0.0162	0.1752	0.6617	0.099

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Table 3. 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}
Te	2*d*	0	0	0	0.02783(7)	0.03037(8)	0.02593(7)	0.00409(6)	0.01171(5)	0.00218(6)
Cl(1)	4*e*	0.25451(6)	–0.00581(4)	0.14994(4)	0.0383(2)	0.0677(3)	0.0386(2)	0.0122(2)	0.0068(2)	–0.0056(2)
Cl(2)	4*e*	–0.11719(6)	0.05060(4)	0.14887(4)	0.0418(2)	0.0530(3)	0.0364(2)	0.0047(2)	0.0189(2)	–0.0030(2)
Cl(3)	4*e*	0.05251(7)	0.16632(4)	–0.03385(6)	0.0559(3)	0.0393(2)	0.0758(4)	0.0043(2)	0.0333(3)	0.0122(3)
N	4*e*	0.0706(2)	0.2278(1)	0.4805(1)	0.0323(7)	0.0329(7)	0.0332(7)	–0.0084(6)	0.0115(6)	–0.0009(6)
C(1)	4*e*	0.0347(2)	0.1256(1)	0.4639(2)	0.0379(9)	0.0353(9)	0.0355(9)	–0.0136(8)	0.0110(8)	–0.0028(7)
C(2)	4*e*	0.1644(2)	0.0604(1)	0.5059(2)	0.0409(9)	0.0338(8)	0.0354(9)	–0.0135(7)	0.0129(7)	–0.0016(7)
C(3)	4*e*	0.2266(3)	0.0376(2)	0.6201(2)	0.059(1)	0.040(1)	0.038(1)	–0.006(1)	0.0162(9)	0.0004(9)
C(4)	4*e*	0.3378(3)	–0.0286(2)	0.6539(2)	0.056(1)	0.049(1)	0.049(1)	–0.004(1)	0.009(1)	0.010(1)
C(5)	4*e*	0.3854(3)	–0.0737(2)	0.5750(2)	0.047(1)	0.052(1)	0.078(2)	0.003(1)	0.022(1)	0.011(1)
C(6)	4*e*	0.3234(3)	–0.0531(2)	0.4617(2)	0.059(1)	0.054(1)	0.068(2)	–0.002(1)	0.036(1)	–0.004(1)
C(7)	4*e*	0.2153(3)	0.0137(1)	0.4271(2)	0.055(1)	0.047(1)	0.041(1)	–0.0065(9)	0.0215(9)	–0.0020(8)
C(10)	4*e*	–0.0746(2)	0.2778(2)	0.4226(2)	0.038(1)	0.049(1)	0.054(1)	–0.0009(9)	0.0141(9)	0.011(1)
C(11)	4*e*	–0.0654(3)	0.3808(2)	0.4339(3)	0.058(2)	0.049(1)	0.089(2)	0.010(1)	0.032(1)	0.019(1)
C(20)	4*e*	0.1939(2)	0.2539(1)	0.4317(2)	0.042(1)	0.040(1)	0.054(1)	–0.0114(8)	0.0251(9)	–0.0004(9)
C(21)	4*e*	0.1545(3)	0.2442(2)	0.3042(2)	0.090(2)	0.063(2)	0.057(2)	–0.022(1)	0.044(1)	–0.002(1)
C(30)	4*e*	0.1275(3)	0.2520(2)	0.6051(2)	0.054(1)	0.041(1)	0.037(1)	–0.0097(9)	0.0108(9)	–0.0087(8)
C(31)	4*e*	0.0174(3)	0.2376(2)	0.6698(2)	0.089(2)	0.073(2)	0.048(1)	–0.008(2)	0.039(1)	–0.007(1)

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