NOTIZEN

The Crystal Structure of $TeCl_3^+AuCl_4^-$

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Tellurium(IV), Gold(III), Crystal Structure, Secondary Interactions

$TeCl_3^+AuCl_4^-$ crystallizes in the triclinic space group $P\bar{1}$ with a = 7.564(2), b = 7.720(3), c = 8.964(3) Å, α = 78.26(3), β = 88.84(3), γ = 89.35(3)°, Z = 2. The structure was refined to R 0.041 for 1380 reflections. The cation polyhedron, including secondary Te···Cl interactions, is a square pyramid with mean Te–Cl 2.294, Te···Cl 3.028 Å. The secondary interactions link the ions to form centrosymmetric $(TeCl_3 \cdot AuCl_4)_2$ dimers.

The structures of salts containing the cations MX_3^+ (M = S, Se, Te; X = halogen) involve characteristic secondary contacts from the central atom M to the accompanying anions. This generally leads to distorted octahedral coordination at M [1]. Only one such structure, $SCl_3^+ICl_4^-$ [2] involves a square-planar anion. We therefore decided to investigate the structures of $MCl_3^+AuCl_4^-$ salts [3]; here we present the structure of the tellurium derivative. Powder data for these compounds have been reported [4]; these data indicate that the compounds are not isostructural.

Experimental

Preparation of $TeCl_3^+AuCl_4^-$. (All reagents and the product are moisture-sensitive and all operations were therefore carried out in a dry-box under N_2. The method is a modification of the original method of Finch *et al.* [3].) 0.02 mmol $TeCl_4$ and 0.01 mmol Au_2Cl_6 were dissolved in 25 ml $AsCl_3$. Dry chlorine was passed through the solution, which was warmed to 40–45 °C. An orange crystalline precipitate formed immediately. After 1 h the chlorine stream was discontinued and the solution heated to 60 °C to redissolve the product. $TeCl_3^+AuCl_4^-$ in the form of orange single crystals (dec. 150 °C) was obtained on slow cooling. The solvent was removed under vacuum.

Crystal structure determination

A crystal 0.25×0.15×0.1 mm was mounted in a glass capillary and used to measure 3480 profile-fitted intensities [5] on a Stoe-Siemens four-circle diffractometer (MoKα radiation, $2\theta_{max}$ 50°). After empirical absorption corrections (ψ-scans), equivalent reflections were merged; of the 1792 unique reflections, 1380 with $F > 4\sigma(F)$ were used for all calculations (program system SHELXTL).

The structure was solved by the heavy-atom method and refined anisotropically to R 0.041, R_w 0.032 (weighting scheme $w = \sigma^{-2}(F)$). See Tables I and II and Fig. 1.

Table I. Atom coordinates (×10⁴) and isotropic temperature factors (Å²×10³).

	x	y	z	U
Au	750(1)	7870(1)	4388.3(.5)	31(1)*
Cl(1)	3682(4)	8377(6)	4646(3)	49(1)*
Cl(2)	464(4)	6618(6)	6911(4)	56(2)*
Cl(3)	−2177(4)	7477(6)	4097(4)	57(2)*
Cl(4)	1054(5)	9141(6)	1870(3)	55(2)*
Te	3209(1)	2326(1)	2274(1)	37(1)*
Cl(5)	4246(5)	5061(6)	2423(4)	61(2)*
Cl(6)	2010(5)	3319(7)	− 76(4)	67(2)*
Cl(7)	5784(4)	1372(6)	1287(4)	59(2)*

* Equivalent isotropic U calculated from anisotropic U.

Table II. Bond lengths (Å) and angles (deg.).

Au–Cl(1)	2.281(4)	Au–Cl(2)	2.278(4)
Au–Cl(3)	2.266(4)	Au–Cl(4)	2.279(4)
Te···Cl(2′)	3.005(5)	Te···Cl(4″)	3.052(5)
Cl(5)–Te	2.291(6)	Cl(6)–Te	2.292(4)
Cl(7)–Te	2.298(5)		
Cl(1)–Au–Cl(2)	91.4(2)	Cl(1)–Au–Cl(3)	177.8(3)
Cl(2)–Au–Cl(3)	89.8(2)	Cl(1)–Au–Cl(4)	88.2(2)
Cl(2)–Au–Cl(4)	179.5(2)	Cl(3)–Au–Cl(4)	90.6(2)
Au–Cl(2)···Te′	103.5(2)	Au–Cl(4)···Te″	97.2(2)
Cl(5)–Te–Cl(6)	93.4(3)	Cl(5)–Te–Cl(7)	95.6(3)
Cl(6)–Te–Cl(7)	93.6(2)	Cl(5)–Te···Cl(2′)	90.7(2)
Cl(6)–Te···Cl(2′)	77.9(2)	Cl(7)–Te···Cl(2′)	169.7(2)
Cl(5)–Te···Cl(4″)	167.0(2)	Cl(6)–Te···Cl(4″)	78.1(2)
Cl(7)–Te···Cl(4″)	94.7(2)	Cl(2′)···Te···Cl(4″)	78.1(2)

Symmetry operators: (′) $-x$, $1-y$, $1-z$; (″) x, $-1+y$, z.

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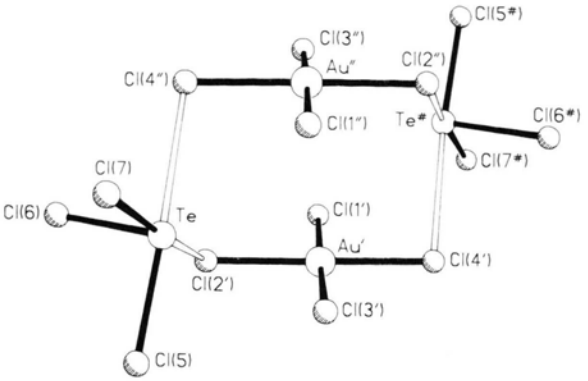

Fig. 1. The dimeric $(TeCl_3 \cdot AuCl_4)_2$ unit, showing the atom numbering scheme. Secondary interactions are indicated by open bonds. Symmetry operators: (') $-x, 1-y, 1-z$; (") $x, -1+y, z$; (#) $-x, -y, 1-z$.

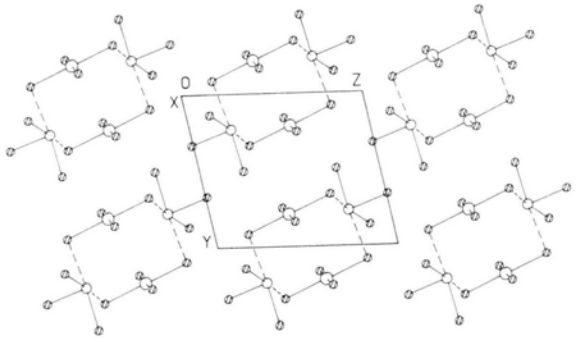

Fig. 2. Projection of the structure of $TeCl_3^+AuCl_4^-$ down the x axis. Atom key: large open circles Au, small open circles Te, shaded circles Cl. Secondary interactions are indicated by broken lines.

Crystal data

$AuCl_7Te$, M = 572.7, triclinic, $P\bar{1}$, a = 7.564(2), b = 7.720(3), c = 8.964(3) Å, α = 78.26(3), β = 88.84(3), γ = 89.35(3)°, V = 512.5 Å^3, Z = 2, D_x = 3.71 g cm^{-3}, F(000) = 500, μ(MoKα) = 18.9 mm^{-1}*.

Discussion

In the $TeCl_3^+$ cation, the average Te–Cl bond length is 2.294 Å and the average Cl–Te–Cl angle 94.2°; these are normal values [1]. The extended geometry is however unexpected; two short Te···Cl contacts (3.005, 3.052 Å) are formed and the idealized overall geometry at tellurium is square pyramidal, leading to the formation of dimeric $(TeCl_3 \cdot AuCl_4)_2$ units with crystallographic inversion symmetry. The next longest Te···Cl contacts (two of 3.363 Å) involve anion chlorines of the same dimeric unit.

The anions display the expected square planar geometry (r.m.s. deviation of five atoms from best plane: 0.016 Å) with a normal average Au–Cl bond length of 2.276 Å [6]. There are no weak axial Au···Cl contacts. The Au–Cl bonds to those chlorine atoms involved in the shorter secondary interactions are not lengthened (although all anion chlorines are involved in secondary interactions <3.37 Å); neither are the Te–Cl bonds *trans* to these interactions.

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* Further details of the crystal structure determination can be obtained from the Fachinformationszentrum Energie, Physik, Mathematik, D-7514 Eggenstein-Leopoldshafen 2, Fed. Rep. of Germany. Any request should be accompanied by a full literature citation and the registration number CSD 52116.

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