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Acta Cryst. (1987). C**43**, 1674–1675

Thallium(I) Tetrachloroaurate(III)

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(*Received* 19 *February* 1987; *accepted* 2 *April* 1987)

Abstract. TlAuCl$_4$, $M_r = 543\cdot15$, monoclinic, $C2/c$, $a = 12\cdot298\,(3)$, $b = 5\cdot825\,(2)$, $c = 9\cdot681\,(3)$ Å, $\beta = 102\cdot09\,(2)°$, $U = 678\cdot1\,(7)$ Å^3, $Z = 4$, $D_x = 5\cdot32$ Mg m^{-3}, $\mu(\text{Mo }K\alpha) = 45\cdot6$ mm^{-1}, $F(000) = 912$, $T = 293$ K, $\lambda(\text{Mo }K\alpha) = 0\cdot71069$ Å, $R = 0\cdot067$ for 721 unique observed reflections. The Tl atom lies on the twofold axis 0, y, 0·25 and is coordinated by ten chlorines. The Au atom lies on the symmetry centre 0·25, 0·75, 0·5 and displays the usual square-planar coordination. TlAuCl$_4$ and RbAuCl$_4$ are isostructural.

Introduction. As part of our studies of aurate salts, we have investigated the reaction of thallium(I) hydroxide with tetrachloroauric acid. One product settles out as a dark brown precipitate; this was refluxed with distilled water and the resulting solution (pH 4) left to stand. Small yellow crystals formed.

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* (Å$^2 \times 10^3$)

	x	y	z	U_{eq}*
Tl	0	2260 (2)	2500	52 (1)
Au	2500	7500	5000	29 (1)
Cl(1)	620 (3)	7336 (7)	4300 (4)	45 (1)
Cl(2)	2694 (4)	4517 (8)	3550 (5)	50 (2)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2. *Bond lengths* (Å) *and angles* (°)

Au–Cl(1)	2·271 (5)	Au–Cl(2)	2·277 (5)
Cl(1)–Au–Cl(2)	90·9 (2)	Cl(1)–Au–Cl(2^{i})	89·1 (2)
Tl···Cl(1)	3·436 (5)	Tl···Cl(2)	3·511 (5)
Tl···Cl(1^{ii})	3·359 (5)	Tl···Cl(1^{iii})	3·350 (5)
Tl···Cl(2^{iv})	3·583 (5)		

Symmetry operators: (i) $0\cdot5-x$, $1\cdot5-y$, $1-z$; (ii) x, $-1+y$, z; (iii) $-x$, $1-y$, $1-z$; (iv) $-0\cdot5+x$, $-0\cdot5+y$, z.

Experimental. A needle $0\cdot2 \times 0\cdot04 \times 0\cdot02$ mm was mounted in a glass capillary and used to record 2726 profile-fitted intensities (Clegg, 1981) on a Stoe–Siemens four-circle diffractometer with monochromated Mo $K\alpha$ radiation ($2\theta_{\max}$ 60°, quadrants $\pm h+k+l$ and $\pm h-k-l$ and some $\pm h+k-l$ equivalents). Three check reflections showed no significant intensity change. An empirical absorption correction based on azimuthal scans was performed, giving transmission factors 0·18–1·00. Merging equivalents gave 990 unique reflections (R_{int} 0·041); 721 reflections with $F > 4\sigma(F)$ were used for all calculations (program *SHELX*76; Sheldrick, 1976). Index ranges after merging were $|h| \leq 16$, $|k| \leq 8$, $|l| \leq 12$. Cell constants were refined from 2θ values of 47 reflections in the range 19–25°.

The structure was solved by analysis of the Patterson function. Refinement on F (full-matrix) proceeded to R 0·067, wR 0·062 [all atoms anisotropic, weighting scheme $w^{-1} = \sigma^2(F) + 0\cdot0004F^2$, 31 parameters, $S = 1\cdot74$, max. Δ/σ 0·001, max. and min. features in final $\Delta\rho$ map +2·5 (near Au), −3·5 e Å^{-3}]. The rather high R value is probably associated with residual absorption errors from a strongly absorbing (but relatively weakly diffracting) needle-shaped crystal. Atomic scattering factors used were those of *SHELX*. Final atomic coordinates are listed in Table 1, and bond lengths and

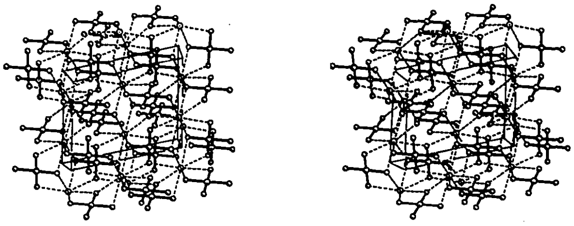

Fig. 1. Stereographic packing plot: view direction slightly rotated from the y axis.

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angles in Table 2.* A stereographic packing plot is given in Fig. 1.

Discussion. $TlAuCl_4$ is isostructural with the corresponding rubidium salt (Strähle & Bärnighausen, 1970). The Au atom displays the expected square-planar coordination; the planarity is exact, since the Au lies on a symmetry centre at 0·25, 0·75, 0·5. The Au—Cl bond lengths [2·271, 2·277 (5) Å] agree well with other salts of the $AuCl_4^-$ anion (Jones, 1981).

The Tl ion lies on a twofold axis, 0, *y*, 0·25, and is coordinated by ten chlorines at distances from 3·35 to 3·58 Å. The coordination geometry corresponds to neither of the idealized forms (bicapped square antiprism or bicapped dodecahedron), since there are three approximately linear Cl···Tl···Cl units. The next longest Tl···Cl contact is 4·38 Å.

As discussed by Strähle & Bärnighausen (1970), the packing of the ions may be considered as a pseudo-hexagonal layer structure.

We thank the Fonds der Chemischen Industrie for financial support.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43935 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Acta Cryst. (1987). C**43**, 1675–1677

Structure (Neutron) of Er_3Al_2

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(*Received* 6 *February* 1986; *accepted* 28 *April* 1987)

Abstract. $M_r = 555\cdot7$, tetragonal, $P4_2/mnm$, $a = 8\cdot1323\ (5)$, $c = 7\cdot5039\ (10)$ Å, $V = 496\cdot3\ (2)$ Å^3, $Z = 4$, $D_x = 7\cdot44$ Mg m^{-3}, $\lambda = 1\cdot237\ (1)$ Å neutrons, μ(calc.) = 0·28 mm^{-1}, $T = 294\ (1)$ K, final $wR = 0\cdot040$ for 953 reflections, 182 independent. At $T = 78\ (1)$ K, 324 reflections, 158 independent, final $wR = 0\cdot080$ same coordinates except *z*(Al) decreased by 0·003 (1), isotropic volume shrinkage approx. 0·9% and lower thermal parameters compared with 294 K values. High-resolution neutron powder diffraction at $T = 294$ K, $\lambda = 1\cdot893$ Å, $\mu R_s = 1\cdot54$, confirmed above results to $wR = 0\cdot064$ from 156 reflections.

Introduction. The only RE_3Al_2 (RE = rare earth) compounds whose structures have been determined are Gd_3Al_2 and Dy_3Al_2, reported (Baenziger & Hegenbarth, 1964) as belonging to space group $P4_2nm$. On the basis of X-ray powder diffraction results Buschow (1965) reported that RE_3Al_2 compounds with RE = Gd, Tb, Dy, Ho or Er are isostructural.

We present here the structure determination of Er_3Al_2 using neutron single-crystal and powder diffraction.

Experimental. (*a*) *Single crystal.* A prismatic crystal 1·50 × 2·75 × 2·61 mm was spark cut from a boule grown by the Czochralski method from 99·9% Er and 99·999% Al at the Laboratoire de Magnétisme, Grenoble, during the tenure by one of us (RKD) of a French Government Scholarship. An adjacent slice of boule was crushed to determine unit-cell parameters by least-squares fit to 17 reflections with $130 < 2\theta < 171°$ using a 114·6 mm diameter Debye–Scherrer camera and Cu $K\alpha$ X-radiation. $\theta/2\theta$ scans, four-circle neutron