operates from a DEC VAX Station 3200 microcomputer. The absorption correction calculated by *XABS* is based on F_o and F_c differences.

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Lists of structure factors and anisotropic displacement parameters have been deposited with the IUCr (Reference: BR1073). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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$K_5InTe_4.KCl$

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Abstract

The structure of the title compound, pentapotassium tetratelluroindate(III)–potassium chloride (1/1), $K_5InTe_4.KCl$, contains isolated $InTe_4^{5-}$ regular tetrahedra which are separated by K^+ and Cl^- ions. This compound may be regarded as a solvated (by KCl) derivative of simple M_5InTe_4 (M = Na, K) compounds, of which the Na (orthorhombic phase) compound only has been structurally characterized to date. The Cl^- anion lying on the z axis of the hexagonal cell is octahedrally surrounded by six K^+ cations.

Comment

Single crystals of $K_5InTe_4.KCl$ have been obtained in the course of preparation of the magnetic material $Fe_5(InTe_4)_2$, discovered by Zhang, van Duyneveldt, Mydosh & O'Connor (1989). So far, single crystals of either K_5InTe_4 or $Fe_5(InTe_4)_2$ have not been obtained (Zhang, Wu & O'Connor, 1993).

The structure shown in Fig. 1 contains discrete tetrahedral $InTe_4^{5-}$ and Cl^- anions, and is closely related to that of orthorhombic *Pbcn* Na_5InTe_4 (Eisenmann, Hofmann & Zagler, 1990), of which it could be considered to be a hexagonal subcell.

Cl^- lies on the z axis and is octahedrally surrounded by six K^+ cations at distances in the range 3.110 (3)–3.194 (3) Å, in agreement with the sum of the ionic radii (1.33 for K^+ and 1.81 Å for Cl^-).

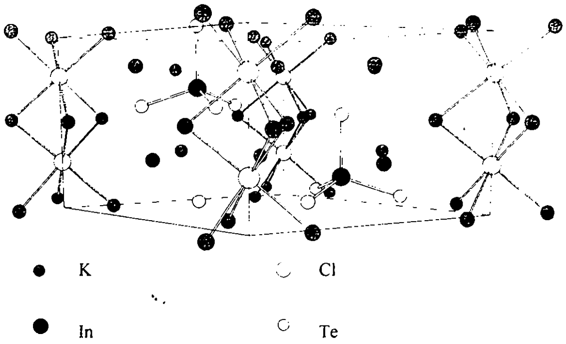

Fig. 1. Packing of $K_5InTe_4.KCl$ in the hexagonal cell.

Experimental

The synthesis was performed in several steps: preparation of K_2Te in liquid ammonia, preparation of amorphous K_5InTe_4 by the melting of appropriate quantities of K_2Te, In and Te in a tantalum crucible at 1223 K and finally reaction of K_5InTe_4 with anhydrous $FeCl_2$ in KBi molten salt.

Crystal data

$K_5InTe_4.KCl$
M_r = 895.26
Hexagonal
$P6_3mc$
a = 11.288 (7) Å
c = 8.013 (2) Å
V = 884.2 (8) Å^3

Mo $K\alpha$ radiation
λ = 0.7107 Å
Cell parameters from 21 reflections
θ = 6.8–20.8°
μ = 9.504 mm^{-1}
T = 298 K

$Z = 2$
$D_x = 3.363$ Mg m^{-3}

Thin plate
$0.28 \times 0.10 \times 0.03$ mm
Dark red

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: empirical (*SHELX76*; Sheldrick, 1976)
$T_{\min} = 0.425$, $T_{\max} = 0.732$
1935 measured reflections
437 independent observed reflections

1837 observed reflections $[I > 3\sigma(I)]$
$R_{\rm int} = 0.026$
$\theta_{\max} = 30°$
$h = 0 \rightarrow 15$
$k = -15 \rightarrow 0$
$l = 0 \rightarrow 11$
3 standard reflections monitored every 60 reflections intensity variation: <3%

Refinement

Refinement on F
$R = 0.0181$
$wR = 0.0227$
$S = 0.912$
437 reflections
27 parameters
$w = 1.7761[\sigma^2(F) + 0.00066F^2]$

$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.58$ e Å^{-3}
$\Delta\rho_{\min} = -1.04$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from Cromer & Mann (1968)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

		x	y	z	$U_{\rm eq}$
In	2(*b*)	1/3	2/3	0.20500	0.0184 (4)
Te(1)	6(*c*)	0.19953 (2)	2*x*	0.0985 (2)	0.0212 (1)
Te(2)	2(*b*)	1/3	2/3	0.5505 (2)	0.0343 (4)
K(1)	6(*c*)	0.1245 (1)	2*x*	0.5186 (3)	0.0324 (8)
K(2)	6(*c*)	0.5209 (1)	2*x*	0.3190 (3)	0.0331 (6)
Cl	2(*a*)	0	0	0.7768 (5)	0.026 (1)

Table 2. *Selected geometric parameters* (Å, °)

In—Te(1)	× 3	2.752 (1)	K(2)—Te(1)	× 2	3.539 (2)
In—Te(2)		2.768 (2)	K(2)—Te(2)		3.571 (2)
K(1)—Cl		3.110 (3)	K(2)—Te(1)	× 2	3.718 (2)
K(1)—Cl		3.194 (3)	K(2)—Te(2)		4.110 (2)
K(1)—Te(1)	× 2	3.472 (2)	Cl—K(1)	× 3	3.110 (3)
K(1)—Te(1)		3.673 (3)	Cl—K(1)	× 3	3.194 (3)
K(1)—Te(2)		4.092 (2)			
Te(1)—In—Te(1)		110.83 (3)	Te(1)—In—Te(2)		108.07 (3)

Statistical tests on intensities were in agreement with a non-centrosymmetric structure and space group $P6_3mc$ (No. 186). The structure was solved using Patterson synthesis and refinements were carried out using the *SHELX76* program (Sheldrick, 1976).

Lists of structure factors and anisotropic displacement parameters have been deposited with the IUCr (Reference: DU1081). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A Scandium Fluorocarbonate, $Ba_3Sc(CO_3)F_7$

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Abstract

Single crystals of barium scandium fluorocarbonate, $Ba_3Sc(CO_3)F_7$, were obtained by hydrothermal growth at high temperature and high pressure. The structure, solved from single-crystal X-ray diffraction data, comprises Ba and Sc polyhedra which form connected layers parallel to (001).

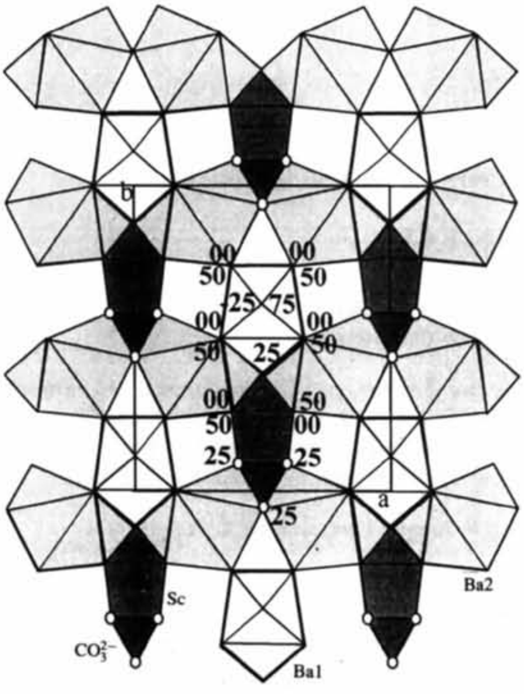

Fig. 1. [001] projection of a layer of Sc and Ba polyhedra at $z = \frac{1}{4}$ in $Ba_3Sc(CO_3)F_7$.