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The $KInTe_2$ Structure Revisited

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Abstract

The framework is built up from $InTe_4$ tetrahedra and KTe_8 square antiprisms. The $InTe_4$ tetrahedra share orthogonal edges to form infinite chains along the *c* axis. These parallel tetrahedral chains are interconnected *via* edge-sharing KTe_8 square antiprisms.

Comment

The tetragonal cell of $KInTe_2$ was first indexed by Franke & Schafer (1972) using the Weissenberg photographic method. Estimated atomic coordinates were given by the authors. The present study reports the single-crystal structure and detailed bond distances and angles for $KInTe_2$.

Crystals of $KInTe_2$ were isolated during studies of the Nd-In-Ti-Te system. The single crystals were grown at 1275 K from a reaction with the target composition $Nd_2In_3Ti_3Te_{12}$. Similar to a method previously reported (Carpenter & Hwu, 1992), the crystal-growth experiment was carried out using an eutectic halide flux ($BaCl_2$/KCl).

A projection onto the *ab* plane of the structure of $KInTe_2$ is shown in Fig. 1. The structure is built up of $InTe_4$ tetrahedra and KTe_8 square antiprisms. Each $InTe_4$ tetrahedron shares edges with two $InTe_4$ tetrahedra along the fourfold screw axis, 4_2, and the four KTe_8 square antiprisms. A chain of $InTe_4$ tetrahedra sharing orthogonal edges can be observed running along the *c* axis. The parallel face-sharing KTe_8 square antiprismatic chains edge-share with the $InTe_4$ tetrahedral chain to form a three-dimensional framework with the TlSe-type structure (Ketelaar, t'Hart, Moerel & Polder, 1939). It should be noted that the title compound is isostructural with $TlInTe_2$ (Müller, Eulenberger & Hahn, 1973). The bond distances and angles of the $InTe_4$ tetrahedra and the KTe_8 square antiprisms are listed in Table 2.

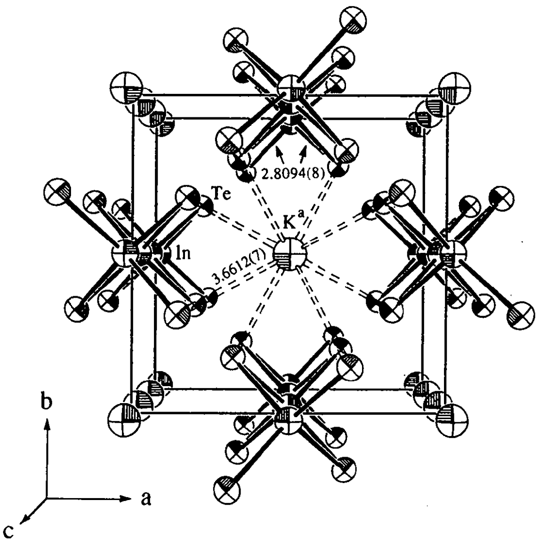

Fig. 1. *ORTEP* (Johnson, 1976) drawing of the $KInTe_2$ structure viewed approximately along the *c* axis. The anisotropic atoms are presented in 90% probability. The bond lengths are given in Å. K^a is at $\frac{1}{2}, \frac{1}{2}, \frac{5}{4}$.

Experimental

Crystal data

$KInTe_2$
$M_r = 409.12$
Tetragonal
$I4/mcm$
$a = 8.598\ (2)$ Å
$c = 7.312\ (3)$ Å
$V = 540.6\ (3)$ Å^3
$Z = 4$
$D_x = 5.027$ Mg m$^{-3$}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 3.35$–$12.05°$
$\mu = 15.52$ mm^{-1}
$T = 296$ K
Needle
$0.7 \times 0.05 \times 0.05$ mm
Dark red

Data collection

Rigaku AFC-5*S* four-circle diffractometer
ω scans
Absorption correction: three azimuthal scans ($2\theta = 11.16, 22.43, 35.30°$)
$T_{\min} = 0.67$, $T_{\max} = 1.00$
208 measured reflections
176 independent reflections

176 observed reflections [$I > 3\sigma(I)$]
$\theta_{\max} = 27.5°$
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 11$
$l = 0 \rightarrow 9$
3 standard reflections monitored at the end of each shell
intensity variation: none detectable

Refinement

Refinement on *F*
Final $R = 0.021$
$wR = 0.032$
$S = 1.61$
176 reflections
10 parameters
$w = [\sigma^2(F_o)]^{-1}$
$(\Delta/\sigma)_{\max} = 0.003$

$\Delta\rho_{\max} = 1.78$ e Å^{-3}
$\Delta\rho_{\min} = -3.43$ e Å^{-3}
Extinction correction: Zachariasen (1968)
Extinction coefficient: $1.9\ (1) \times 10^{-6}$
Atomic scattering factors from Cromer & Waber (1974)

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

$B_{eq} = (8\pi^2/3)$ trace U.

	x	y	z	B_{eq}
K	0.0	0.0	0.25	2.20 (7)
In	0.0	0.5	0.25	1.41 (3)
Te	0.32456 (5)	0.17544*	0.0	1.39 (2)

* $y = \frac{1}{2} - x$.

Table 2. *Important geometry* (Å, °) *for polyhedra in* $KInTe_2$

KTe_8 polyhedron		
$K—Te^{a,b,c,d,e,f,g,h}$	3.6612 (7)	(8×)
$Te^{a/c/e/g}—K—Te^{b/d/f/h}$	120.09 (2)	(4×)
$Te^{a/b/e/f}—K—Te^{c/d/g/h}$	80.68 (2)	(4×)
$Te^{a/b/c/d}—K—Te^{e,f/e,f/g,h/g,h}$	75.56 (1)	(8×)
$Te^{a/b/e/f}—K—Te^{d/c/h/g}$	131.34 (2)	(4×)
$Te^{a/b/c/d}—K—Te^{g/h/f/e}$	67.74 (2)	(4×)
$Te^{a/b/c/d}—K—Te^{h/g/e/f}$	151.33 (2)	(4×)
$InTe_4$ polyhedron		
$In—Te^{e,g,i,j}$	2.8094 (8)	(4×)
$Te^{e/e/g/i}—In—Te^{g/j/i/j}$	115.05 (2)	(4×)
$Te^{e/g}—In—Te^{i/j}$	98.81 (3)	(2×)

Symmetry codes: (*a*) x, y, z; (*b*) $-x, -y, z$; (*c*) $x, -y, \frac{1}{2}+z$; (*d*) $-x, y, \frac{1}{2}+z$; (*e*) $-y, x, z$; (*f*) $y, -x, z$; (*g*) $y, x, \frac{1}{2}+z$; (*h*) $-y, -x, \frac{1}{2}+z$; (*i*) $y, 1-x, z$; (*j*) $-y, 1-x, \frac{1}{2}+z$.

On the basis of the intensity statistics, as well as the successful solution and structure refinements, the space group was determined to be *I4/mcm* (No. 140).

Data reduction: *TEXSAN PROCESS* (Molecular Structural Corporation, 1985). Program(s) used to solve structure: *TEXSAN*. Program(s) used to refine structure: *TEXSAN*. The atomic coordinates were found by direct methods using *SHELXS86* (Sheldrick, 1985).

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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 71217 (5 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: ST1049]

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Structure of Dimeric Dichloro(4,4′-dimethyl-2,2′-bipyridine)copper(II) Hemihydrate

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Abstract

The crystal consists of discrete dimeric units, di-μ-chloro-bis[chloro(4,4′-dimethyl-2,2′-bipyridine)copper(II)] hydrate, linked to one water molecule and to another unit by van der Waals forces. Each dimeric unit contains a Cu_2Cl_2 core surrounded by two chlorine ions and two 4,4′-dimethyl-2,2′-bipyridine ligands. The geometry about each Cu atom is best described as a distorted trigonal bipyramid. The basal plane contains the N(2) atom of 4,4′-dimethyl-2,2′-bipyridine, the Cl(2*a*) atom that bridges the two monomers, and the Cl(1) ion. The two axial sites are occupied by the N(1) atom and the Cl(2) ion.

Comment

The present work continues structural studies of Cu^{II} complexes with diimines. The dichloro(4,4′-dimethyl-2,2′-bipyridine)copper(II) complex has been

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