Crystal structure of tetrapotassium hexatellurodistannate, $K_4Sn_2Te_6$

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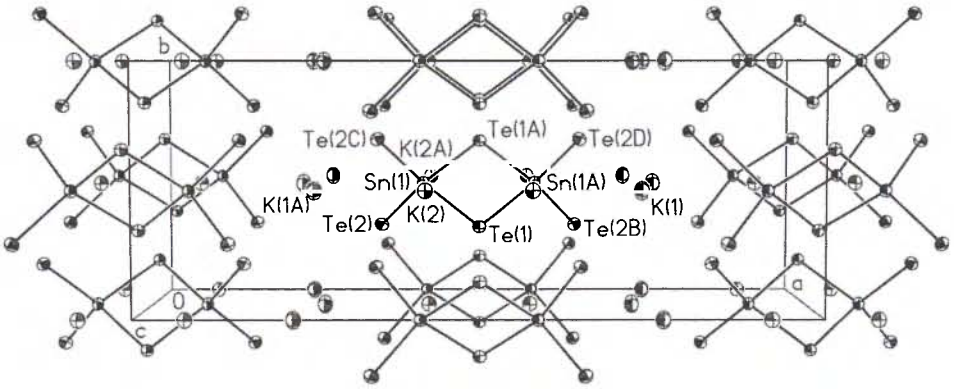
Received February 16, 2000, CSD-No. 409483



Abstract

$K_4Sn_2Te_6$, orthorhombic, *Cmca* (No. 64), $a = 23.1511(4)$ Å, $b = 8.6277(1)$ Å, $c = 8.6536(2)$ Å, $V = 1728.5$ Å^3, $Z = 4$, $R_{gt}(F) = 0.030$, $wR_{gt}(F^2) = 0.065$, $T = 170$ K.

Source of material

85.0 mg (0.666 mmol) Te, 19.8 mg (0.167 mmol) Sn, and 30.8 mg (0.222 mmol) La were reacted in an evacuated fused silica ampoule at 1098 K for 150 hours. The product was ground up and combined with 101.9 mg (0.221 mmol) K_2Te_3 and reacted in a fused silica ampoule at 798 K for 150 hours. This resulted in bronze colored plates of $K_4Sn_2Te_6$.

Discussion

$K_4Sn_2Te_6$ is not isostructural with the triclinic $K_4Sn_2Se_6$ structure [1], but contains the same $(Sn_2Te_6)^{4-}$ anions composed of edge-sharing $SnTe_4$ tetrahedra. The bond length of the terminal Sn—Te(t) bonds is 2.737 Å and the bridging Sn—Te(b) bond length is 2.834 Å. The Te(b)–Sn–Te(b) bond angle is constrained to 92.22° from an ideal tetrahedral angle.

Table 1. Data collection and handling.

Crystal:	bronze plate, size 0.06 × 0.06 × 0.02 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	137.42 cm^{-1}
Diffractometer, scan mode:	Bruker CCD, ω
$2\theta_{max}$:	56.46°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5356, 1092
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 953
$N(param)_{refined}$:	32
Program:	SHELXTL [2]

Table 2. 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(1)	8*f*	0	0.16699(6)	0.33277(6)	0.0129(3)	0.0115(3)	0.0102(3)	0	0	0.0005(2)
Te(2)	16*g*	0.14995(2)	0.18693(4)	0.68702(4)	0.0147(2)	0.0134(2)	0.0113(2)	–0.0013(2)	–0.0015(1)	–0.0007(1)
Sn(1)	8*d*	0.08485(2)	0	1/2	0.0108(3)	0.0127(3)	0.0110(3)	0	0	–0.0015(2)
K(1)	8*d*	0.26583(9)	0	1/2	0.016(1)	0.0251(9)	0.025(1)	0	0	–0.0057(8)
K(2)	8*d*	–0.07738(8)	1/2	1/2	0.016(1)	0.0181(9)	0.015(1)	0	0	0.0002(7)

Acknowledgments. The authors thank NSF grant CHE-9625378 for financial support, and S. M. Miller for crystallographic help.

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References

1. Eisenmann, B.; Hansa, J.: Crystal structure of tetrapotassium hexaselenodistannate, $K_4Sn_2Se_6$. Z. Kristallogr. **203** (1993) 299-300.
2. Bruker SHELXTL. Structure Determination Programs. Version 5.03, Bruker AXS, Inc., Madison, Wisconsin, USA 1994.