Crystal structure of potassium calcium bismuthide, KCaBi

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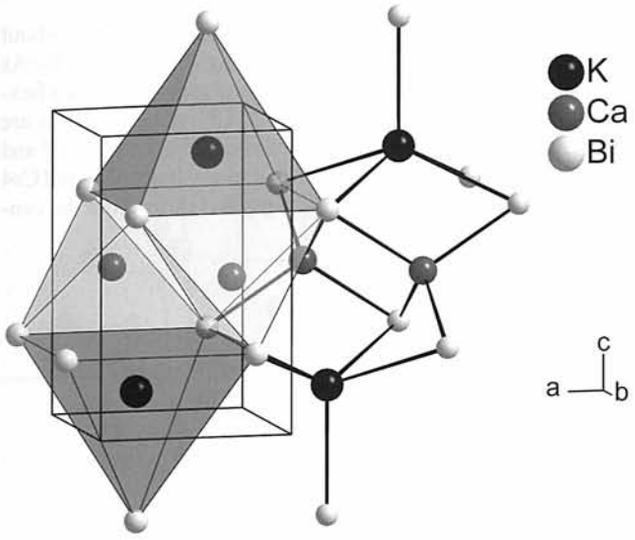

Abstract

BiCaK, tetragonal, *P4/nmm* (No. 129), $a = 5.384(1)$ Å, $c = 8.380(2)$ Å, $V = 242.9$ Å^3, $Z = 2$, $R_{gt}(F) = 0.027$, $wR_{ref}(F^2) = 0.067$, $T = 293$ K.

Source of material

The compound was synthesized from a stoichiometric mixture of the elements in a sealed steel-tube which was filled under inert gas (Ar). To ensure homogenization the sample was first heated up to a complete melt at 870 K (one week). Well shaped single crystals of the air sensitive compound were obtained after subsequent annealing at 570 K (three weeks).

Discussion

In the course of our work on alkali pnictide we tried to preparate new ternary pnictides with alkali and alkaline earth metals. KCaBi belongs to the Cu_2Sb (PbClF) structure familiy [1] and is an example for the small subgroup of ternary pnictides with alkali and alkaline earth metals [2-4]. The structure can be characterized by layers of condensed $CaBi_4$ tetrahedra (d(Ca—Bi) = 3.212(1) Å) alternating along [001] with layers of K atoms. The arrangement of Bi atoms corresponds to a cubic close packing with half of the tetrahedral holes filled by Ca in an ordered way. The K atoms do not occupy the centers of the octahedral holes but are shifted along [001] into a square-pyramidal coordination of Bi atoms (d(K—Bi) = 3.569(5) Å; 4.025(2) Å).

Table 1. Data collection and handling.

Crystal:	grey metallic plate, size 0.05 × 0.2 × 0.3 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	379.89 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS, φ
$2\theta_{max}$:	63.16°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	412, 271
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 253
$N(param)_{refined}$:	10
Programs:	SHELXL-97 [5] DIAMOND [6]

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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}
K	2*c*	1/4	1/4	0.8651(6)	0.081(3)	U_{11}	0.025(2)	0	0	0
Ca	2*b*	3/4	1/4	1/2	0.0176(8)	U_{11}	0.021(1)	0	0	0
Bi	2*c*	1/4	1/4	0.29090(6)	0.0200(3)	U_{11}	0.0163(3)	0	0	0

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