Z. Kristallogr. NCS 213 (1998) 455–456

Crystal structures of rubidium calcium arsenide, RbCaAs and of rubidium calcium antimonide, RbCaSb

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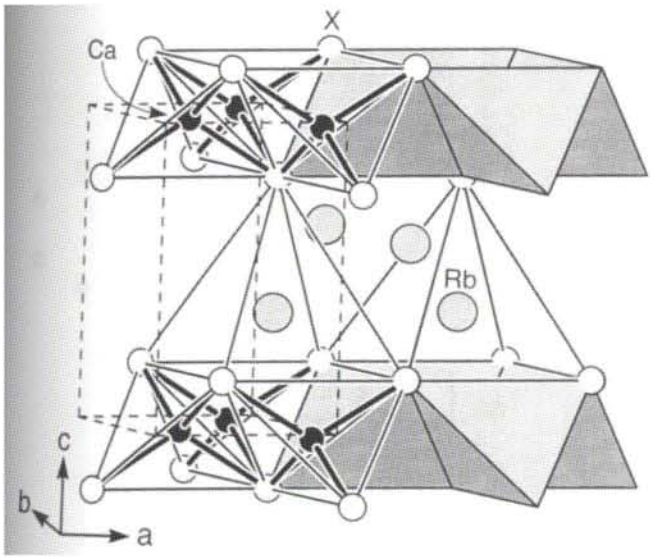
Received December 16, 1997, transferred to 2nd update of database ICSD in 1998, CSD-No. 409177 and 409178

1. Rubidium calcium arsenide, RbCaAs



Source of material: The title compounds were synthesized from stoichiometric amounts of the elements (Rb:Ca:As(Sb) = 1:1:1) in sealed niobium ampoules in evacuated quartz tubes at 973 K.

RbCaAs and RbCaSb are isostructural with KMnAs (see ref. 1). The structure can be described as an elongated *ccp* arrangement of As or Sb atoms along [101]. Half of the tetrahedral holes are centered by Ca atoms. The filled tetrahedra share edges forming $^{2}_{\infty}[CaX_{4/4}]^{1-}$ layers (X = As, Sb) parallel (001) with d(Ca–As) = 296.4 pm and d(Ca–Sb) = 315.8 pm. These layers are held together by the Rb atoms, which are displaced from the centers of the octahedra resulting in a pyramidal coordination (CN = 5). The band gaps from diffuse reflexion spectra E_g = 2.4 eV (RbCaAs) and E_g = 2.3 eV (RbCaSb) are in agreement with the ruby-red color of these compounds.

AsCaRb, tetragonal, *P4/nmm* (No. 129), a =5.142(1) Å, c =7.932(2) Å, V =209.7 Å^3, Z =2, $R(F)$ =0.032, $R_w(F^2)$ =0.062.

Table 1. Parameters used for the X-ray data collection

Crystal:	ruby-red platelet, size 0.08 x 0.08 x 0.02 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	206.08 cm^{-1}
Diffractometer:	Stoe STADI4
Scan mode:	ω
$T_{measurement}$:	293 K
$2\theta_{max}$:	65°
N(hkl)$_{unique}$:	261
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
N($param$)$_{refined}$:	10
Program:	SHELXL-93

Table 2. Final 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}
Rb	2c	1/4	1/4	0.6262(2)	0.0478(4)	U_{11}	0.0236(8)	0	0	0
Ca	2a	3/4	1/4	0	0.0163(5)	U_{11}	0.0206(9)	0	0	0
As	2c	1/4	1/4	0.1860(2)	0.0185(3)	U_{11}	0.0180(6)	0	0	0

2. Rubidium calcium antimonide, RbCaSb

CaRbSb, tetragonal, *P4/nmm* (No. 129), a =5.363(2) Å, c =8.469(1) Å, V =243.6 Å^3, Z =2, $R(F)$ =0.037, $R_w(F^2)$ =0.083.

Table 3. Parameters used for the X-ray data collection

Crystal:	ruby-red platelet, size 0.08 x 0.08 x 0.02 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	164.30 cm^{-1}
Diffractometer:	Stoe STADI4
Scan mode:	ω
$T_{measurement}$:	293 K
$2\theta_{max}$:	65°
N(hkl)$_{unique}$:	296
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
N($param$)$_{refined}$:	10
Program:	SHELXL-93

Table 4. Final 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}
Rb	2*c*	1/4	1/4	0.6343(2)	0.0439(5)	U_{11}	0.0237(6)	0	0	0
Ca	2*a*	3/4	1/4	0	0.0163(5)	U_{11}	0.0194(9)	0	0	0
Sb	2*c*	1/4	1/4	0.1970(1)	0.0175(3)	U_{11}	0.0153(4)	0	0	0

References

1. Linowsky, L.; Bronger, W.: Synthese und Kristallstruktur von KMnP und KMnAs. Z. Anorg. Allg. Chem. **409** (1974) 221-227.
2. Sheldrick, G. M.: SHELXL-93, a program for refining crystal structures. University of Göttingen, Germany 1993.