Refinement of the crystal structure of dirubidium trithioargentate(I), $Rb_2Ag_4S_3$

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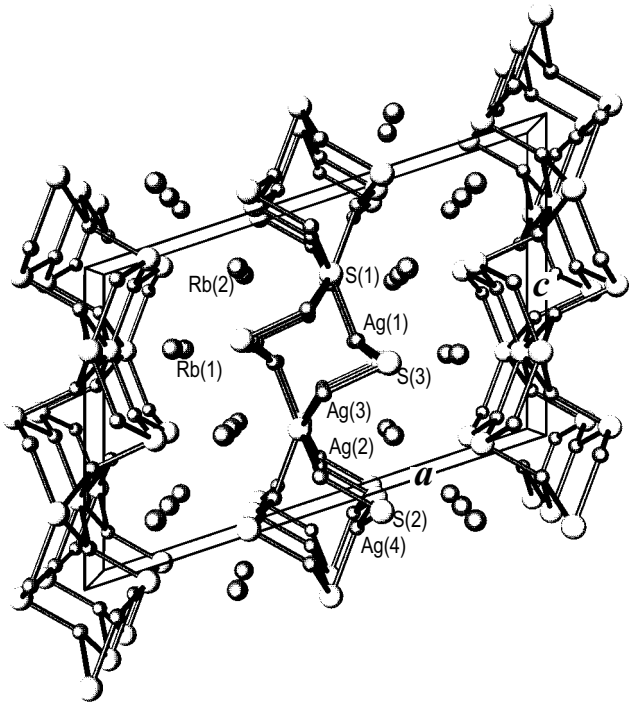

Abstract

$Ag_4Rb_2S_3$, monoclinic, $C12/m1$ (No. 12), a = 17.808(8) Å, b = 4.310(2) Å, c = 11.799(5) Å, β = 108.55(2)°, V = 858.6 Å^3, Z = 4, $R_{gt}(F)$ = 0.038, $wR_{obs}(F)$ = 0.038, T = 294 K.

Source of material

$Rb_2Ag_4S_3$ was prepared by reacting a stoichiometric mixture of Rb_2S, Ag (99.99 %) and S (99.9%) powders in an evacuated silica ampoule. The sample was gradually heated to 1070 K, annealed for three days and finally brought to ambient temperature at a controlled cooling rate of 2 K/h.

Discussion

The structure of $Rb_2Ag_4S_3$ is characterized by the formation of infinite anionic layers $[Ag_4S_3]$ which run parallel to (001). The present single crystal investigation corroborates an earlier assignment of $Rb_2Ag_4S_3$ to the $K_2Ag_4S_3$ type which was based on Guinier powder data [1].

Table 1. Data collection and handling.

Crystal:	black metallic prism, size 0.10 × 0.10 × 0.15 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	204.94 cm^{-1}
Diffractometer, scan mode:	Enraf Nonius CAD4, $\omega/2\theta$
$2\theta_{max}$:	53.92°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1226, 1064
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 3\ \sigma(I_{obs})$, 912
$N(param)_{refined}$:	56
Programs:	MULTAN [2] MolEN [3], DIFABS [4], ATOMS [5]

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}
Rb(1)	4*i*	0.18999(8)	0	0.8434(1)	0.0129(6)	0.0174(8)	0.0132(5)	0	0.0048(4)	0
Rb(2)	4*i*	0.33114(8)	0	0.6592(1)	0.0156(6)	0.0172(8)	0.0140(5)	0	0.0058(4)	0
Ag(1)	4*i*	0.40986(7)	0	–0.00895(9)	0.0176(5)	0.0155(6)	0.0178(4)	0	0.0045(4)	0
Ag(2)	4*i*	0.00979(7)	0	0.37546(9)	0.0163(5)	0.0371(8)	0.0208(5)	0	0.0007(4)	0
Ag(3)	4*i*	0.01713(7)	0	0.13260(9)	0.0175(5)	0.0247(7)	0.0217(4)	0	0.0104(3)	0
Ag(4)	4*i*	0.41051(8)	0	0.4111(1)	0.0362(7)	0.0150(7)	0.0283(5)	0	0.0069(5)	0
S(1)	4*i*	0.4660(2)	0	0.2250(3)	0.017(2)	0.010(2)	0.010(1)	0	0.004(1)	0
S(2)	4*i*	0.1379(2)	0	0.5399(3)	0.014(2)	0.010(2)	0.013(1)	0	–0.001(1)	0
S(3)	4*i*	0.1523(2)	0	0.1070(3)	0.016(1)	0.005(2)	0.018(1)	0	0.010(1)	0

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