

Crystal structure of trirubidium tetracopper(I) dithulium(III) tridecaboride, $\text{Rb}_3\text{Cu}_4\text{Tm}_2\text{Br}_{13}$

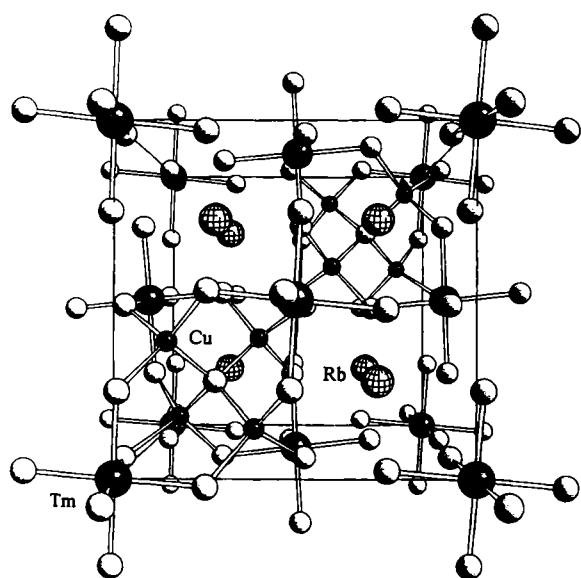
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Source of material: Single crystals were obtained by cooling a mixture of RbBr , CuBr and TmBr_3 (molar ratio 3:4:2) in a sealed quartz tube under strict exclusion of moisture and oxygen from 873 K to room temperature during two weeks.

$\text{Rb}_3\text{Cu}_4\text{Tm}_2\text{Br}_{13}$ crystallizes isostructurally with $(\text{NH}_4)_3\text{Cu}_4\text{Ho}_2\text{Br}_{13}$ (see ref. 1). The structure may be derived from the fluorite type of structure, where $[\text{TmBr}_6]$ octahedra are approximately cubically closest packed like in CaF_2 . The $[\text{BrCu}_4]$ tetrahedra fill one quarter and Rb^+ three quarters of the tetrahedral sites.

$\text{Br}_{13}\text{Cu}_4\text{Rb}_3\text{Tm}_2$, cubic, $Pn\bar{3}$ (No. 201), $a = 11.0148(7)$ Å, $V = 1336.4$ Å³, $Z = 2$, $R(F) = 0.044$, $R_w(F^2) = 0.099$.

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

Crystal:	colorless, square prism, size 0.1 x 0.1 x 0.1 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	337.54 cm ⁻¹
Diffractometer:	Stoe \AA PD5
Scan mode:	100 plates, $\Delta\phi = 1^\circ$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	56.32°
$N(hkl)_{\text{unique}}$:	560
Criterion for I_o :	$I_o > 2\sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	19
Program:	SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Tm	4b	0	0	0	0.0347(3)	U_{11}	U_{11}	-0.0004(2)	U_{12}	U_{12}
Cu	8e	0.3779(1)	x	x	0.0608(6)	U_{11}	U_{11}	0.0007(7)	U_{12}	U_{12}
Rb	6d	1/4	3/4	3/4	0.054(1)	0.103(2)	0.072(1)	0	0	0
Br(1)	24h	0.4858(1)	0.2515(1)	0.9741(1)	0.0575(6)	0.0337(5)	0.0547(6)	-0.0032(5)	0.0087(4)	0.0006(4)
Br(2)	2a	1/4	1/4	1/4	0.0453(7)	U_{11}	U_{11}	0	0	0

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References

1. Wickleder, M. S.; Bohnsack, A.; Meyer, G.: Synthese und Kristallstruktur von $(\text{NH}_4)_3\text{Cu}_4\text{Ho}_2\text{Br}_{13}$. Weitere Bromide vom Typ $(\text{NH}_4)_3\text{Cu}_4\text{M}_2\text{Br}_{13}$ (M=Dy-Lu, Y) und $\text{Rb}_3\text{Cu}_4\text{Ho}_2\text{Br}_{13}$. Z. Anorg. Allg. Chem. **622** (1996) 675-678.
2. Sheldrick, G. M.: SHELXL-93, a program for refining crystal structures. University of Göttingen, Germany 1993.