Crystal structure of trirubidium tetracopper(I) dithulium(III) tridecabromide, $Rb_3Cu_4Tm_2Br_{13}$

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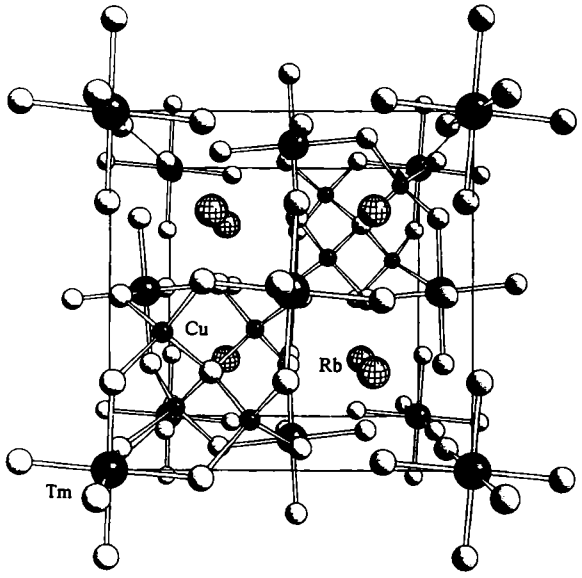

Source of material: Single crystals were obtained by cooling a mixture of RbBr, CuBr and $TmBr_3$ (molar ratio 3:4:2) in a sealed quartz tube under strict exclusion of moisture and oxygen from 873 K to room temperature during two weeks.

$Rb_3Cu_4Tm_2Br_{13}$ crystallizes isostructurally with $(NH_4)_3Cu_4Ho_2Br_{13}$ (see ref. 1). The structure may be derived from the fluorite type of structure, where $[TmBr_6]$ octahedra are approximately cubically closest packed like in CaF_2. The $[BrCu_4]$ tetrahedra fill one quarter and Rb^+ three quarters of the tetrahedral sites.

$Br_{13}Cu_4Rb_3Tm_2$, cubic, $Pn\bar{3}$ (No. 201), a =11.0148(7) Å, V =1336.4 Å^3, 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 IPDS
Scan mode:	100 plates, Δ φ =1°
$T_{measurement}$:	293 K
$2\theta_{max}$:	56.32°
$N(hkl)_{unique}$:	560
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	19
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}
Tm	4*b*	0	0	0	0.0347(3)	U_{11}	U_{11}	–0.0004(2)	U_{12}	U_{12}
Cu	8*e*	0.3779(1)	x	x	0.0608(6)	U_{11}	U_{11}	0.0007(7)	U_{12}	U_{12}
Rb	6*d*	1/4	3/4	3/4	0.054(1)	0.103(2)	0.072(1)	0	0	0
Br(1)	24*h*	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)	2*a*	1/4	1/4	1/4	0.0453(7)	U_{11}	U_{11}	0	0	0

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References

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2. Sheldrick, G. M.: SHELXL-93, a program for refining crystal structures. University of Göttingen, Germany 1993.