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Crystal structure of copper iron rhenium molybdenium sulfide, $(Cu_{0.85}Fe_{0.15})(Re_{2.85}Mo_{1.15})S_8$

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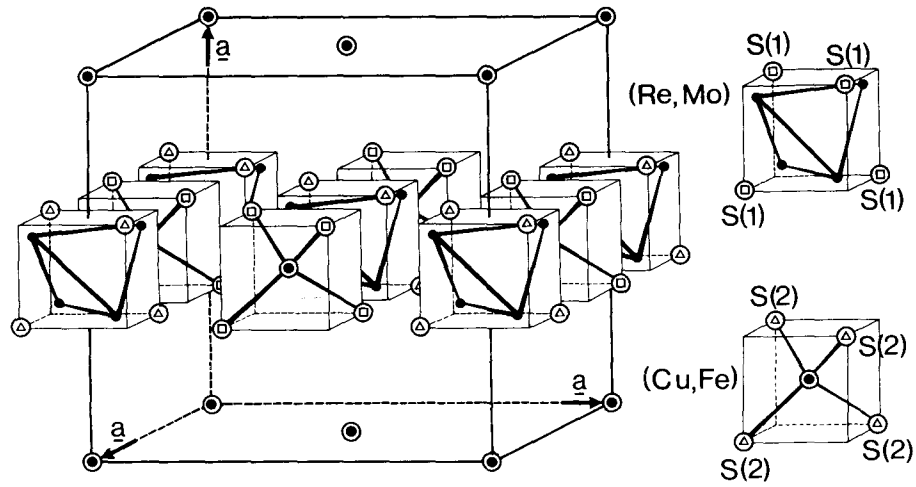

Source of material: see ref. 4.
The structure of the synthetic mineral is closely related to a normal (2,3) spinel structure of the type $[A_2]T[B_4]OS_8$ with space group $Fd\bar{3}m$. Vacancies on the tetrahedral sites and shifts of B and S atoms cause a symmetry reduction to space group $F\bar{4}3m$. The B atoms are statistically substituted by Re and Mo forming tetrahedral clusters with a metal-metal distance of 2.822(2) Å.

Cubic, $F\bar{4}3m$ (no 216), $a = 9.5715(5)$ Å, $V = 876.9$ Å^3, $Z = 4$, $R = 0.040$.

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

Diffractometer type:	Siemens R3M/V	Number of unique reflections:	233
Wave length:	Mo K_α radiation (0.7107 Å)	Criterion for unobserved reflections:	$F_o < 3\sigma(F_o)$
Crystal characteristics:	black crystal, size $0.022 \times 0.019 \times 0.015$ mm	Number of refined parameters:	13
		Scan mode:	2Θ-Θ scan
Temperature of measurement:	293 K	μ:	337.8 cm^{-1}
$2\theta_{max}$:	70°	Structure solution program used:	PROMETHEUS

Table 2. Final atomic coordinates and displacement parameters (in $Å^2$)

Atom	x	y	z	U_{iso}/U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Re	0.39577(6)	0.39577(6)	0.39577(6)	0.0046(2)	0.0046(2)	0.0046(2)	−0.0002(3)	−0.0002(3)	−0.0002(3)
Mo	0.39577(6)	0.39577(6)	0.39577(6)	0.0046(2)	0.0046(2)	0.0046(2)	−0.0002(3)	−0.0002(3)	−0.0002(3)
S(1)	0.6364(4)	0.6364(4)	0.6364(4)	0.006(2)	0.006(2)	0.006(2)	−0.0009(9)	−0.0009(9)	−0.0009(9)
S(2)	0.1349(4)	0.1349(4)	0.1349(4)	0.006(2)	0.006(2)	0.006(2)	−0.0012(9)	−0.0012(9)	−0.0012(9)
Cu	0.0	0.0	0.0	0.010(1)	0.010(1)	0.010(1)	0.0	0.0	0.0
Fe	0.0	0.0	0.0	0.010(1)	0.010(1)	0.010(1)	0.0	0.0	0.0

Further details of the structure determination (e.g. structure factors) have been deposited within the relevant database and can be accessed as Collection No. 300242 or ordered from the Fachinformationszentrum Karlsruhe, D-7514 Eggenstein-Leopoldshafen.

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