Crystal structure of hexastrontium dodecacopper tridecairon heptacosasulfide, $\text{Sr}_6\text{Cu}_{12}\text{Fe}_{13}\text{S}_{27}$

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Source of material: The title compound was prepared by heating at 1173 K under sulfur atmosphere SrS and CuFeS_2 in molar ratio 1:2.

The title compound is isostructural to $\text{Ba}_6\text{Cu}_{12}\text{Fe}_{13}\text{S}_{27}$ (see ref. 1) and djerfisherite (see ref. 2). It is built up of edge and corner sharing MS_4 ($\text{M} = \text{Cu}$ and Fe) tetrahedra which form large interconnecting tunnels and octahedral cages. One $[\text{FeS}_6]$ and $[\text{Ba}_6\text{S}]$ octahedra per unit cell are located in these channels and cages, respectively.

Table 2. Final atomic coordinates and displacement parameters (in $\text{\AA}^2$)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sr(1)	6f	1/2	1/2	0.7990(1)	0.0186(6)	U_{11}	0.0150(7)	0	0	0
Fe(1)	1a	0	0	0	0.015(1)	U_{11}	U_{11}	0	0	0
Fe(2)	24m	0.30	0.86180(7)	x	0.6380(1)	0.0185(5)	0.0239(6)	-0.0020(4)	-0.0005(3)	U_{13}
Cu(2)	24m	0.20	0.86180(7)	x	0.6380(1)	0.0185(5)	0.0239(6)	-0.0020(4)	-0.0005(3)	U_{13}
S(1)	1b	1/2	1/2	1/2	0.015(2)	U_{11}	U_{11}	0	0	0
S(2)	8g	0.2892(2)	x	x	0.0159(7)	U_{11}	U_{11}	0.0012(7)	U_{12}	U_{12}
S(3)	6e	0	0	0.7584(4)	0.017(1)	U_{11}	0.013(2)	0	0	0
S(4)	12h	0	1/2	0.7382(3)	0.016(1)	U_{11}	0.014(1)	0	0	0

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

Crystal:	black lump, size 0.2 x 0.2 x 0.15 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 $\text{\AA}$)
μ :	189.30 cm^{-1}
Diffractometer:	Siemens P4
Scan mode:	ω
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	296
Criterion for F_o :	$F_o > 3 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	24
Program:	SHELXTL-plus

$\text{Cu}_{12}\text{Fe}_{13}\text{S}_{27}\text{Sr}_6$, cubic, $Pm\bar{3}m$ (No. 221), $a = 10.203(1)$ $\text{\AA}$, $V = 1062.1$ $\text{\AA}^3$, $Z = 1$, $R(F) = 0.041$, $R_w(F) = 0.037$.

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References

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