Crystal structure of pentamercury dialuminum octaselenide, $Hg_5Al_2Se_8$

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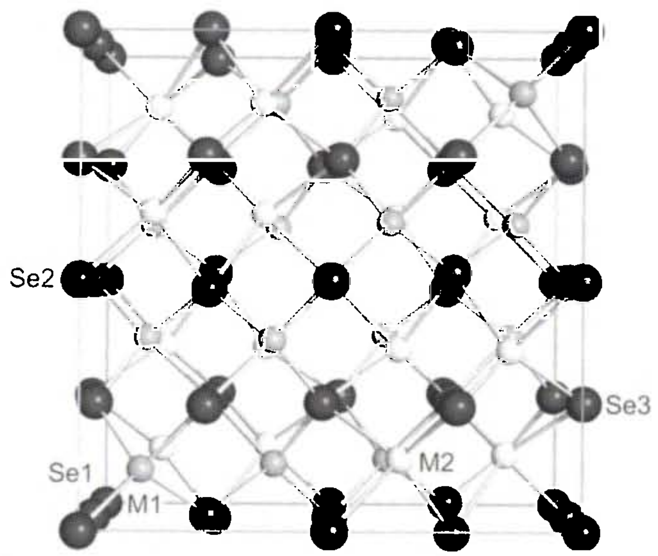
Received July 17, 2001, CSD-No. 409566



Abstract

$Al_2Hg_5Se_8$, cubic, $F\bar{4}3m$ (No. 216), a = 11.704(1) Å, V = 1603.3 Å^3, Z = 4, $R(P)$ = 0.070, $wR(P)$ = 0.093, $R(I)$ = 0.122, T = 293 K.

Source of material

Microcrystalline powder of $Hg_5Al_2Se_8$ was synthesized by chemical vapour transport starting from HgSe, Al and Se in molar ratio of 5:2:3 and $AlCl_3$ as transport agent in a vertical two zone furnace.

Experimental details

To determine the structure, an initial structure model was set up by plausibility considerations and refined by the Rietveld method. The site occupation of the cations was refined by alternately setting free the thermal and the occupancy parameters. With respect to the chemical composition, the given idealized values for the occupation parameters were obtained [1].

Table 1. Data collection and handling.

Powder:	dark grey
Wavelength:	Cu K_α radiation (1.5406 Å)
μ:	1041.5 cm^{-1}
Diffractometer, scan mode:	Stoe STADI P, transmission
$2\theta_{max}$, stepwith:	119.98°, 0.02°
$N(points)_{measured}$:	5489
$N(hkl)_{measured}$:	89
$N(param)_{refined}$:	9
Program:	GSAS [3]

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Discussion

The title compound crystallises with an eightfold superstructure of the sphalerite structure [1]. The close structural relationship to the sphalerite structure can easily be seen in the figure.

The superstructure results from the cation distribution in the two different sphalerite subcells. Following the rules for tetrahedral structures [2], there is one vacancy per formula unit present in the structure ($\square Hg_5Al_2Se_8$). Within the group of $A_5B_2X_8$ chalcogenides, $Hg_5Al_2Se_8$ forms a new structural variant.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
Se(1)	4a	0	0	0	0.052(5)
Se(2)	4b	0	1/2	0	0.020(4)
Se(3)	24g	1/4	1/4	0.0179(3)	0.064(2)
M(1)[a]	16e	0.1178(2)	x	x	0.033(2)
M(2)[b]	16e	0.1391(2)	x	x+1/2	0.049(1)

a: M(1) = 0.375Hg + 0.375Al
b: M(2) = 0.875Hg + 0.125Al

Acknowledgment. We thank the Deutsche Forschungsgemeinschaft for financial support.

References

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3. Larson, A. C.; von Dreele, R. B.: GSAS - General Structure Analysis System. Los Alamos National Laboratory, USA 2000.