Crystal structure of indium monosulfide, InS, *at 7.9 GPa*

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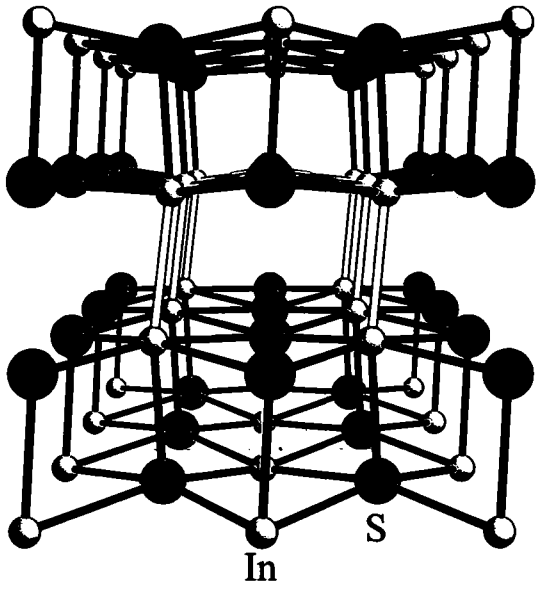

Abstract

InS, monoclinic, $P12_1/n1$ (No. 14), $a = 3.8630(8)$ Å, $b = 10.7668(9)$ Å, $c = 3.8554(7)$ Å, $\beta = 90.880(7)°$, $V = 160.3$ Å^3, $Z = 4$, $wR(P) = 0.120$, $R(I) = 0.062$, $T = 295$ K, $P = 7.9$ GPa.

Source of material

The starting material were dark red pieces of InS ingots. Powdering was performed by grinding of the crystalline material at ambient conditions.

Experimental details

High pressures were generated using gasketed diamond anvil cells with a 4:1 methanol/ethanol mixture as a pressure transmitting medium. For pressure calibration we used the ruby luminescence method.

Discussion

The figure shows the crystal structure of a high-pressure modification of InS in a projection along the *a* axis. Both atom types, indium and sulphur, realise a distorted octahedron as a first coordination sphere. The crystal structure is a distorted variety of the tetragonal calomel type. It can be described as slightly distorted NaCl-type double-layers which are interconnected by homonuclear In bonds. In comparison to the orthorhombic low-pressure modification, the inclination angle between the In-dumbbells and the long axis is pronouncedly reduced in the monoclinic high-pressure phase. The selected non-standard setting $P2_1/n$ points out the metrical relationship of tetragonal HgCl and orthorhombic as well as monoclinic InS. Detailed discussions of the crystal chemical similarities of InS, HgCl, GeS, and TlI have been given earlier [1-3]. The present results [space group No. 14, standard setting $P2_1/c$; $a = 386.25(1)$ pm, $b = 1076.6(1)$ pm, $c = 5.4991(4)$, $\beta = 135.488(8)°$; In (0.018(3), 0.1189(5), –0.037(2)), S (0.02(1), 0.359(1), 0.000(6))] are in disagreement with earlier work which supposes hp-InS to crystallize in the tetragonal space group *I4/mmm* [4].

Table 1. Data collection and handling.

Powder:	dark red
Wavelength:	synchrotron radiation (0.4654 Å)
μ:	12.5 cm^{-1}
Diffractometer:	Daresbury Station 9.1, φ scan, transmission
$2\theta_{max}$, stepwidth:	26°, 0.02°
$N(points)_{measured}$:	1001
$N(hkl)_{measured}$:	108
$N(param)_{refined}$:	9
Programs:	CSD [5], ATOMS [6]

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

Atom	Site	x	y	z	U_{iso}
In	4*e*	0.055(2)	0.1191(4)	–0.038(2)	0.0143(3)
S	4*e*	0.019(5)	0.359(1)	–0.001(6)	0.0139(5)

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