

# Refinement of the crystal structure of Sb-I, at 2.22 GPa

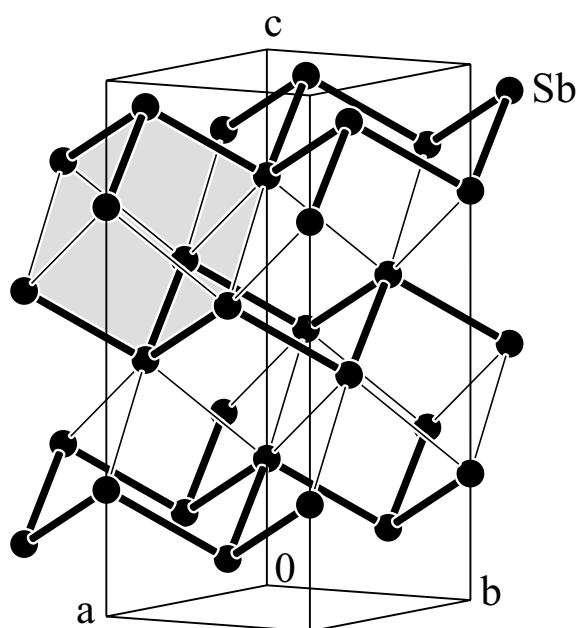
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## Abstract

Sb, trigonal,  $R\bar{3}m$  (No. 166),  $a = 4.2687(2)$  Å,  $c = 10.9244(6)$  Å,  $V = 172.4$  Å<sup>3</sup>,  $Z = 6$ ,  $R(P) = 0.066$ ,  $R(I) = 0.059$ ,  $T = 295$  K,  $P = 2.22$  GPa.

## Source of material

Antimony of 99.999% purity (ABCR GmbH, Germany) was used for the experiments. Polycrystalline samples were obtained by grinding of antimony shots at ambient conditions.

## Experimental details

Angle-dispersive X-ray powder diffraction experiments were performed on ID-9 at ESRF using an image plate detector. The powdered particles were placed in a gasketed diamond anvil high-pressure cell using a small sphere of ruby for pressure calibration and a 4:1 mixture of ethanol and methanol as a pressure transmitting medium.

**Table 2.** Atomic coordinates and displacement parameters (in Å<sup>2</sup>).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>11</sub>	<i>U</i> <sub>22</sub>	<i>U</i> <sub>33</sub>	<i>U</i> <sub>12</sub>	<i>U</i> <sub>13</sub>	<i>U</i> <sub>23</sub>
Sb	6c	0	0	0.2362(1)	0.038(5)	<i>U</i> <sub>11</sub>	0.046(9)	<i>U</i> <sub>11</sub> /2	0	0

## Discussion

Structural parameters of antimony at elevated pressures up to 8.5 GPa were determined earlier by means of single crystal X-ray diffraction in diamond anvil cells [1]. We re-refined the parameter values in order to gain a quantitative measure for the reliability of full profile refinements using powder patterns measured with synchrotron radiation. The result of the least squares procedure is within three standard deviations identical to the values obtained by single crystal diffraction methods ( $z = 0.2358(6)$  at  $P = 1.5$  GPa and  $z = 0.2379(6)$  at  $P = 2.66$  GPa [1]). The resulting interatomic distances of  $3 \times 2.895(1)$  Å and  $3 \times 3.253(1)$  Å support the finding that the rhombohedral low-pressure phase approaches a simple cubic arrangement with increasing pressures [1,2].

**Table 1.** Data collection and handling.

Powder:	black, size 5–10 μm
Wavelength:	synchrotron radiation (0.41844 Å)
$\mu$ :	75.0 cm <sup>-1</sup>
Diffractometer:	MAR3450
$2\theta_{\text{max}}$ , stepwidth	24.9°, 0.01
$N(\text{points})_{\text{measured}}$ :	2304
$N(hkl)_{\text{measured}}$ :	35
$N(\text{param})_{\text{refined}}$ :	4
Programs:	WinCSD [3], ImageIntegrator [4]

## References

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