Zeitschrift für Kristallographie 205, 327 – 328 (1993)


# Crystal structure of lead silver tribismuth sulfide, $PbAgBi_3S_6$

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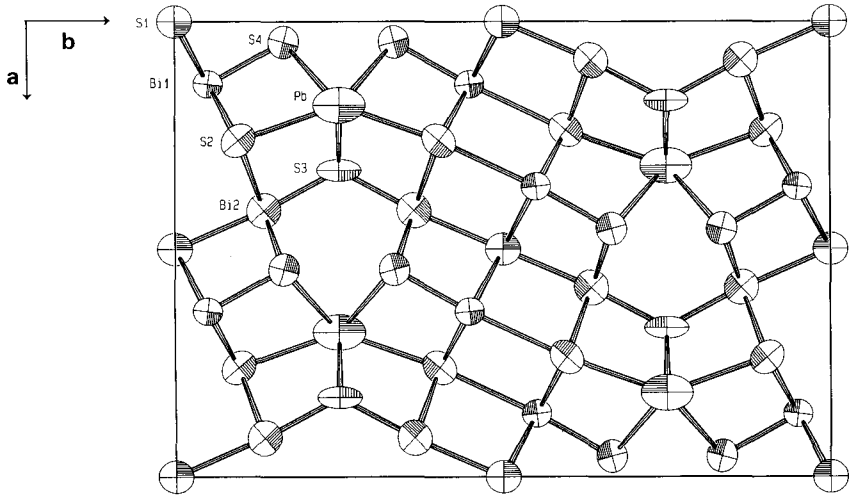
(Received August 12, 1992, transferred to database ICSD November 15, 1992)




Synthesis: The sulfide was prepared by recristallization in silica tubes at 770 K. Strong differences between weighted R-value and unit weighted R-value are caused by very small crystals and few observed reflections. Therefore the residual electron density was also calculated based on the observed reflections only. Natural gustavite show Ag-Bi-ordering (Steins et al., 1991), whereas synthetic gustavite show statistical distribution.

Orthorhombic, Cmcm (No. 63), $a = 4.077(2)$, $b = 13.477(7)$, $c = 19.88(2)$ Å, V = 1092.3 Å$^3$, Z = 4, R = 0.076.

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

| | | | |
|---|---|---|---|
| Diffractometer type: | Siemens-Stoe | Number of unique reflections: | 1376 |
| Wave length: | Mo $K_\alpha$ radiation (0.7107 Å) | Criterion for unobserved reflections: | $F_o < 1.5\sigma(F_o)$ |
| Crystal characteristics: | lamina, size $0.08 \times 0.032 \times 0.0005$ mm | Number of refined parameters: | 39 |
| | | Scan mode: | $\omega/\Theta$ |
| Temperature of measurement: | 288 K | $\mu$: | 670.315 $cm^{-1}$ |
| $2\theta_{max}$: | 70° | Structure solution program used: | ORXFLS3 |

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

| Atom | $x$ | $y$ | $z$ | $U_{iso}/U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|
| Pb | 0.0 | 0.1835(2) | 0.25 | 0.025(1) | 0.031(2) | 0.070(3) | 0.0 | 0.0 | 0.0 |
| Bi(1) | 0.5 | 0.1377(1) | 0.0502(1) | 0.0188(7) | 0.0186(8) | 0.022(1) | 0.0 | 0.0008(9) | 0.0 |
| Bi(2) | 0.5 | 0.4150(2) | 0.3645(1) | 0.023(1) | 0.030(1) | 0.030(2) | 0.0 | 0.003(1) | 0.0 |
| S(1) | 0.0 | 0.0 | 0.0 | 0.016(6) | 0.026(9) | 0.03(1) | 0.0 | 0.0 | 0.0 |
| S(2) | 0.0 | 0.2612(9) | 0.0968(7) | 0.023(4) | 0.028(6) | 0.030(6) | 0.0 | −0.011(6) | 0.0 |
| S(3) | 0.5 | 0.327(1) | 0.25 | 0.029(8) | 0.012(7) | 0.05(1) | 0.0 | 0.0 | 0.0 |
| S(4) | 0.5 | 0.0450(9) | 0.1659(6) | 0.018(5) | 0.026(6) | 0.024(7) | 0.0 | −0.001(5) | 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. 300265 or ordered from the Fachinformationszentrum Karlsruhe, D-7514 Eggenstein-Leopoldshafen.

**References:**

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