

$\text{Pb}_7(\text{S}_{0.33}\text{Br}_{0.67})_6\text{Br}_6$ *hP24*(176) $P6_3/m - h^4$ **Pb₇S₂Br₁₀** [1]

Structural features: Infinite columns of base-linked $\text{Pb}[\text{Br}_4(\text{Br,S})_2][\text{Br}(\text{Br,S})]$ bicapped trigonal prisms ($\text{Pb}[\text{Br}_5(\text{Br,S})_3]$ square antiprisms) share atoms to form a 3D-framework with WC-type columns (3 prisms in the triangular cross-section); additional Pb in channels of hexagonal cross-section parallel to [001] (displaced from the axis, partial disorder). Variant of Th_7S_{12} .

Krebs B. (1973) [1]

 $\text{Br}_{10}\text{Pb}_7\text{S}_2$ $a = 1.2273$, $c = 0.4319$ nm, $c/a = 0.352$, $V = 0.5634$ nm³, $Z = 1$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|------------|-------------|----------|----------|---------------|-------|----------------------------------|
| Pb1 | 6 <i>h</i> | <i>m</i> .. | 0.0217 | 0.0295 | $\frac{1}{4}$ | 0.167 | |
| Br2 | 6 <i>h</i> | <i>m</i> .. | 0.1391 | 0.51851 | $\frac{1}{4}$ | | square pyramid Pb ₅ |
| M3 | 6 <i>h</i> | <i>m</i> .. | 0.23013 | 0.23949 | $\frac{1}{4}$ | | single atom Pb |
| Pb4 | 6 <i>h</i> | <i>m</i> .. | 0.41899 | 0.1398 | $\frac{1}{4}$ | | square antiprism Br ₈ |

 $\text{M3} = 0.667\text{Br} + 0.333\text{S}$ Transformation from published data: origin shift $0\ 0\ \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $wR = 0.054$, $T = 293$ K

Remarks: We assigned an approximate value to the Br/S ratio of site M3 based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Krebs B. (1973), *Z. Anorg. Allg. Chem.* 396, 137-151.