

CuBr	<i>hP6</i>	(186) $P6_3mc - b^2a$
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**CuBr  $\beta$**  [1]

Structural features: Close-packed Br layers in h stacking; main part of Cu in tetrahedral, some Cu in octahedral voids.

Krug J., Sieg L. (1952) [1]

BrCu

$a = 0.406$ ,  $c = 0.666$  nm,  $c/a = 1.640$ ,  $V = 0.0951$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Br1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.25		tetrahedron Cu <sub>4</sub>
Cu2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.625	0.9	7-vertex polyhedron Br <sub>4</sub> Cu <sub>3</sub>
Cu3	$2a$	$3m.$	0	0	0.0	0.1	9-vertex polyhedron Cu <sub>3</sub> Br <sub>6</sub>

Transformation from published data: origin shift 0 0 0.75

Experimental: powder, film, X-rays

Remarks: Phase stable at  $664 < T < 743$  K. We deduced the space group from the coordinates of all the atoms in the unit cell.

References: [1] Krug J., Sieg L. (1952), Z. Naturforsch. A 7, 369-371.