

$\text{Cu}_{0.7}\text{Zn}_2$	$hP3$	(187) $P\text{-}6m2$ – eda
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**CuZn<sub>3</sub> ht** [1]

Structural features:  $\text{CuZn}_6\text{Zn}_3$  tricapped trigonal prisms share atoms to form a dense 3D-framework (partial vacancies).

Lenz J., Schubert K. (1971) [1]

$\text{Cu}_{0.70}\text{Zn}_2$

$a = 0.4275$ ,  $c = 0.259$  nm,  $c/a = 0.606$ ,  $V = 0.0410$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Cu1	1e	-6m2	$\frac{2}{3}$	$\frac{1}{3}$	0	0.7	pentacapped trigonal prism $\text{Zn}_9\text{Cu}_2$
Zn2	1d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		rhombic dodecahedron $\text{Zn}_8\text{Cu}_6$
Zn3	1a	-6m2	0	0	0		pentacapped trigonal prism $\text{Cu}_3\text{Zn}_8$

Transformation from published data ( $P\text{-}6$ ): origin shift  $\frac{2}{3} \frac{1}{3} \frac{1}{2}$

Experimental: powder, film, X-rays, T = 873 K

Remarks: The description in space group (174)  $P\text{-}6$  in [1] does not take into consideration all symmetry elements of the proposed structure.

References: [1] Lenz J., Schubert K. (1971), Z. Metallkd. 62, 810-816.