

CuI	<i>hP6</i>	(187) <i>P-6m2</i> – igda
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# **CuI $\beta$** [1]

Structural features: Close-packed I layers in h stacking; Cu in octahedral (displaced towards a face) and tetrahedral voids (partial disorder).

Bührer W., Hälg W. (1977) [1]

CuI

$a = 0.4300$ ,  $c = 0.7207$  nm,  $c/a = 1.676$ ,  $V = 0.1154$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cu1	2 <i>i</i>	3 <i>m.</i>	$\frac{2}{3}$	$\frac{1}{3}$	0.29	0.3	
Cu2	2 <i>g</i>	3 <i>m.</i>	0	0	0.39	0.7	
I3	1 <i>d</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		
I4	1 <i>a</i>	-6 <i>m2</i>	0	0	0		8-vertex polyhedron Cu <sub>8</sub>

Experimental: powder, diffractometer, neutrons, R = 0.150, T = 653 K

Remarks: Phase stable at  $640 < T < 680$  K. Supersedes a report on  $\beta$ -CuI with ZnO-type (ZnS wurtzite) structure in [2]. Short interatomic distances for partly occupied site(s); impossibly short distances occur for published site occupancies.

References: [1] Bührer W., Hälg W. (1977), *Electrochim. Acta* 22, 701-704. [2] Miyake S., Hoshino S., Takenaka T. (1952), *J. Phys. Soc. Jpn.* 7, 19-24.