| CuI | *hP*8 | (187) *P*-6*m*2 – hg$^2$ed |
|---|---|---|

**CuI β** [1]
Structural features: Close-packed I layers in h stacking; Cu in tetrahedral, octahedral, and near trigonal voids (partial disorder).

Yude Y. et al. (1990) [1]
CuI
$a$ = 0.4288, $c$ = 0.7189 nm, $c/a$ = 1.677, $V$ = 0.1145 nm$^3$, $Z$ = 2

| site | Wyck. | sym. | $x$ | $y$ | $z$ | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| Cu1 | 2*h* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.11 | 0.70 | |
| Cu2 | 2*g* | 3*m*. | 0 | 0 | 0.09 | 0.15 | |
| Cu3 | 2*g* | 3*m*. | 0 | 0 | 0.24 | 0.15 | |
| I4 | 1*e* | -6*m*2 | $^2/_3$ | $^1/_3$ | 0 | | |
| I5 | 1*d* | -6*m*2 | $^1/_3$ | $^2/_3$ | $^1/_2$ | | 8-vertex polyhedron $Cu_8$ |

Transformation from published data: origin shift $^2/_3$ $^1/_3$ $^1/_2$
Experimental: powder, diffractometer, neutrons, $wR_p$ = 0.160, T = 598 K

Remarks: Phase stable at 640 < T < 680 K; sample containing also the rt modification γ-CuI. Refinement of the occupancies of the I sites showed no significant deviation from unity. Short interatomic distances for partly occupied site(s); impossibly short distances occur for published site occupancies.

References: [1] Yude Y., Boysen H., Schulz H. (1990), Z. Kristallogr. 191, 79-91.