Cu_3P	*hP*24	(185) $P6_3cm$ – c^3ba

Cu_3P [1], Strukturbericht notation $D0_{21}$; Na_3As α [2]; $AuCd_3$ hexagonal [3]; LaF_3 [7]
Structural features: Puckered hexagon-mesh Cu_2 and approximately planar hexagon-mesh CuP layers alternate along [001]. $P(Cu_6Cu_5)$ pentacapped trigonal prisms in h stacking share atoms to form a dense 3D-framework.

Olofsson O. (1972) [1]
$Cu_{2.84}P$
$a = 0.69593$, $c = 0.7143$ nm, $c/a = 1.026$, $V = 0.2996$ nm^3, $Z = 6$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
P1	6*c*	..*m*	0.3322	0	0.0713		pseudo Frank-Kasper Cu_{11}
Cu2	6*c*	..*m*	0.3761	0	0.3967	0.936	pseudo Frank-Kasper P_4Cu_9
Cu3	6*c*	..*m*	0.7194	0	0.2448	0.900	anticuboctahedron P_4Cu_8
Cu4	4*b*	3..	$^1/_3$	$^2/_3$	0.1215		icosahedron P_3Cu_9
Cu5	2*a*	3.*m*	0	0	0.0		icosahedron P_3Cu_9

Transformation from published data: -*x*,-*y*,-*z*; origin shift 0 0 0.6787
Experimental: single crystal, diffractometer, X-rays, R = 0.037

Remarks: The structure type (antitype) was originally proposed for LaF_3 (tysonite) [7], however, the structure of LaF_3 was (re)determined in space group (165) *P*-3*c*1 ([5]; [9]). On the contrary, structure proposals for Cu_3P in space group (165) *P*-3*c*1 ([4]; [5]) are superseded in [1]; the author states that also Cu_3As may crystallize in space group (185) $P6_3cm$. The structure proposal for α-Na_3As in space group (194) $P6_3/mmc$ with $^1/_3$ cell volume in [6] is also superseded (see [2] and [8]). Strukturbericht notation $D0_{21}$ was defined on the superseded structure proposal for Cu_3P.

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