$Cu_3P_4S_4I_3$	*hP*84	(185) $P6_3cm - d^4c^6$

$(CuI)_3P_4S_4$ [1]
Structural features: P_4S_4 cage molecules (one P_3S, one P_3S_3 and two P_3S_2 rings) share vertices with chains of vertex-linked $Cu(PI_3)$ tetrahedra to form a 3D-framework.

Reiser S. et al. (2002) [1]
$Cu_3I_3P_4S_4$
a = 1.9082, c = 0.6691 nm, c/a = 0.351, V = 2.1099 nm^3, Z = 6

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
I1	12*d*	1	0.1986	0.53194	0.36872		non-coplanar triangle Cu_3
S2	12*d*	1	0.22096	0.324	0.3458		non-colinear P_2
Cu3	12*d*	1	0.3332	0.53916	0.2663		tetrahedron PI_3
P4	12*d*	1	0.33631	0.4276	0.3543		tetrahedron S_2CuP
Cu5	6*c*	..*m*	0.12585	0	0.0977		tetrahedron PI_3
I6	6*c*	..*m*	0.13279	0	0.4889		non-coplanar triangle Cu_3
P7	6*c*	..*m*	0.2372	0	0.0		tetrahedron S_3Cu
S8	6*c*	..*m*	0.3052	0	0.2467		non-colinear P_2
P9	6*c*	..*m*	0.4008	0	0.0991		non-coplanar triangle SP_2
S10	6*c*	..*m*	0.5894	0	0.148		non-colinear P_2

Transformation from published data: origin shift 0 0 0.7182
Experimental: twinned crystal, diffractometer, X-rays, R = 0.032, T = 273 K

References: [1] Reiser S., Brunklaus G., Hong J.H., Chan J.C.C., Eckert H., Pfitzner A. (2002), Chem. Eur. J. 8, 4228-4233.