

Cu₃P₄Se₄I₃*hP*96(185) *P*6₃*cm* – d⁵c⁶**(CuI)₃P₄Se₄** [1]

Structural features: P₄Se₄ cage molecules (one P₃Se, one P₃Se₃ and two P₃Se₂ rings) share vertices with chains of vertex-linked Cu(PI₃) tetrahedra (partial disorder) to form a 3D-framework. Variant of (CuI)₃P₄S₄ with partly disordered arrangement of Cu.

Pfitzner A., Reiser S. (1999) [1]

Cu₃I₃P₄Se₄*a* = 1.9601, *c* = 0.67196 nm, *c/a* = 0.343, *V* = 2.2358 nm³, *Z* = 6

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
I1	12 <i>d</i>	1	0.20185	0.53358	0.11357		6-vertex polyhedron Cu ₆
Se2	12 <i>d</i>	1	0.21648	0.32459	0.15037		non-colinear P ₂
Cu3	12 <i>d</i>	1	0.335	0.5413	0.20627	0.445	
Cu4	12 <i>d</i>	1	0.336	0.5417	0.01847	0.555	
P5	12 <i>d</i>	1	0.3382	0.4311	0.11317		
Cu6	6 <i>c</i>	.. <i>m</i>	0.12356	0	0.38757		tetrahedron PI ₃
I7	6 <i>c</i>	.. <i>m</i>	0.12944	0	0.0		non-coplanar triangle Cu ₃
P8	6 <i>c</i>	.. <i>m</i>	0.2327	0	0.48577		tetrahedron Se ₃ Cu
Se9	6 <i>c</i>	.. <i>m</i>	0.29987	0	0.21637		non-colinear P ₂
P10	6 <i>c</i>	.. <i>m</i>	0.3978	0	0.37927		non-coplanar triangle SeP ₂
Se11	6 <i>c</i>	.. <i>m</i>	0.57942	0	0.33417		non-colinear P ₂

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.29893Experimental: single crystal, diffractometer, X-rays, *R* = 0.059, *T* = 298 K

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Pfitzner A., Reiser S. (1999), *Inorg. Chem.* 38, 2451-2454.