

Cu_8GeSe_6	$hP90$	$(185) P6_3cm - d^4c^5b^2a^2$
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Cu_8GeSe_6 rt [1]

Structural features: Se forms a tetrahedrally close-packed (MgZn₂-type) framework; Ge in tetrahedral, Cu in trigonal and tetrahedral voids. Single GeSe_4 tetrahedra.

Jaulmes S. et al. (1991) [1]

Cu_8GeSe_6

$a = 1.2648$, $c = 1.176$ nm, $c/a = 0.930$, $V = 1.6292$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	12d	1	0.1291	0.4991	0.2379		8-vertex polyhedron Se_4Cu_4
Se2	12d	1	0.1562	0.487	0.0314		square pyramid GeCu_4
Cu3	12d	1	0.1979	0.3361	0.1282		bicapped square prism Se_4Cu_6
Cu4	12d	1	0.1996	0.3535	0.365		8-vertex polyhedron Se_4Cu_4
Se5	6c	$\bar{3}m$	0.1805	0	0.0467		4-vertex polyhedron GeCu_3
Cu6	6c	$\bar{3}m$	0.1851	0	0.257		7-vertex polyhedron Se_3Cu_4
Se7	6c	$\bar{3}m$	0.3419	0	0.3737		octahedron Cu_6
Cu8	6c	$\bar{3}m$	0.5525	0	0.0564		8-vertex polyhedron Se_4Cu_4
Se9	6c	$\bar{3}m$	0.6402	0	0.2446		monocapped trigonal prism Cu_7
Se10	4b	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.2831		tetrahedron GeCu_3
Ge11	4b	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.4819		tetrahedron Se_4
Ge12	2a	3.m	0	0	0.0		tetrahedron Se_4
Se13	2a	3.m	0	0	0.302		tetrahedron GeCu_3

Transformation from published data: origin shift 0 0 0.198

Experimental: single crystal, diffractometer, X-rays, $wR = 0.043$, $T = 293$ K

Remarks: Phase stable at $T < 328$ K. The structure was refined in 4D-superspace with commensurate modulation $q = (a^* + b^*)/3$ in [2].

References: [1] Jaulmes S., Julien Pouzol M., Laruelle P., Rivet J. (1991), Acta Crystallogr. C 47, 1799-1803. [2] Onoda M., Ishii M., Pattison P., Shibata K., Yamamoto A., Chapuis G. (1999), J. Solid State Chem. 146, 355-362.