Cu_8GeSe_6	*hP*38	(186) $P6_3mc$ – $c^5b^2a^2$

Cu_8GeSe_6 ht [1]
Structural features: Se forms a tetrahedrally close-packed ($MgZn_2$-type) framework; Ge in tetrahedral, Cu in tetrahedral and trigonal voids (partial disorder for the latter). Single $GeSe_4$ tetrahedra.

Jaulmes S. et al. (1991) [1]
$Cu_{7.94}GeSe_6$
a = 0.7307, c = 1.175 nm, c/a = 1.608, V = 0.5433 nm^3, Z = 2

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Cu1	6*c*	.*m*.	0.437	0.563	0.256	0.333	
Cu2	6*c*	.*m*.	0.4668	0.5332	0.327	0.657	
Cu3	6*c*	.*m*.	0.5293	0.4707	0.088	0.657	
Cu4	6*c*	.*m*.	0.8137	0.1863	0.457		7-vertex polyhedron Se_3Cu_4
Se5	6*c*	.*m*.	0.8218	0.1782	0.249		
Se6	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.083		9-vertex polyhedron Cu_9
Se7	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.45		
Se8	2*a*	3*m*.	0	0	0.0		tetrahedron $GeCu_3$
Ge9	2*a*	3*m*.	0	0	0.1979		tetrahedron Se_4

Experimental: single crystal, diffractometer, X-rays, wR = 0.047, T = 350 K

Remarks: Phase stable at T > 328 K. Short interatomic distances for partly occupied site(s).

References: [1] Jaulmes S., Julien Pouzol M., Laruelle P., Rivet J. (1991), Acta Crystallogr. C 47, 1799-1803.