

Cu_8GeSe_6	$hP32$	$(186) P6_3mc - c^4b^2a^2$
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Cu_8GeSe_6 ht [1]

Structural features: Se forms a tetrahedrally close-packed (MgZn₂-type) framework; Ge in tetrahedral, Cu in tetrahedral and trigonal voids (partial disorder for the latter). Single GeSe₄ tetrahedra.

Onoda M. et al. (1999) [1]

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$a = 0.73164$, $c = 1.17679$ nm, $c/a = 1.608$, $V = 0.5455$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	$6c$	$.m.$	0.462	0.538	0.306	0.667	tetrahedron Se ₃ Cu
Cu2	$6c$	$.m.$	0.528	0.472	0.096		monocapped trigonal prism Se ₄ Cu ₃
Cu3	$6c$	$.m.$	0.813	0.187	0.454		coplanar triangle Se ₃
Se4	$6c$	$.m.$	0.821	0.179	0.249		pentagonal pyramid GeCu ₅
Se5	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.084		octahedron Cu ₆
Se6	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.45		trigonal prism Cu ₆
Se7	$2a$	$3m.$	0	0	0.0		tetrahedron GeCu ₃
Ge8	$2a$	$3m.$	0	0	0.202		tetrahedron Se ₄

Experimental: powder, diffractometer, X-rays, synchrotron, $wR_p = 0.074$, $T = 350$ K

Remarks: Phase stable at $T > 328$ K.

References: [1] Onoda M., Ishii M., Pattison P., Shibata K., Yamamoto A., Chapuis G. (1999), J. Solid State Chem. 146, 355-362.