

GaSe	<i>hP</i> 16	(186) $P6_3mc - b^4a^4$
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GaSe δ [1]

Structural features: Close-packed Se layers in AABBAACC stacking; Ga₂ dumbbells in trigonal prismatic voids. Se₃Ga-GaSe₃ units share vertices to form infinite slabs. Layer structure with sandwiches consisting of four sublayers (Se-Ga-Ga-Se).

Kuhn A. et al. (1975) [1]

GaSe

$a = 0.3755$, $c = 3.1990$ nm, $c/a = 8.519$, $V = 0.3906$ nm³, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ga1	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.0338		tetrahedron Se ₃ Ga
Ga2	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.1099		tetrahedron GaSe ₃
Se3	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.2474		non-coplanar triangle Ga ₃
Se4	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.3971		non-coplanar triangle Ga ₃
Se5	2 <i>a</i>	3 <i>m.</i>	0	0	0.0000		non-coplanar triangle Ga ₃
Se6	2 <i>a</i>	3 <i>m.</i>	0	0	0.1493		non-coplanar triangle Ga ₃
Ga7	2 <i>a</i>	3 <i>m.</i>	0	0	0.2839		tetrahedron Se ₃ Ga
Ga8	2 <i>a</i>	3 <i>m.</i>	0	0	0.3613		tetrahedron Se ₃ Ga

Transformation from published data: origin shift 0 0 0.1781

Experimental: single crystal, diffractometer, X-rays, R = 0.098

Remarks: Preliminary data in [2].

References: [1] Kuhn A., Chevalier R., Rimsky A. (1975), Acta Crystallogr. B 31, 2841-2842. [2] Kuhn A., Chevy A., Chevalier R. (1975), Phys. Status Solidi A 31, 469-475.