

GaSe	<i>hP8</i>	(187) <i>P-6m2 – ihg²</i>
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GaSe 2H [2]

Structural features: Close-packed Se layers in CCAA stacking; Ga₂ dumbbells in trigonal prismatic voids (stacking sequence CaaC AbbA). Se₃Ga-GaSe₃ units share vertices to form infinite slabs. Layer structure with sandwiches consisting of four sublayers (Se-Ga-Ga-Se). See Fig. IV.12.

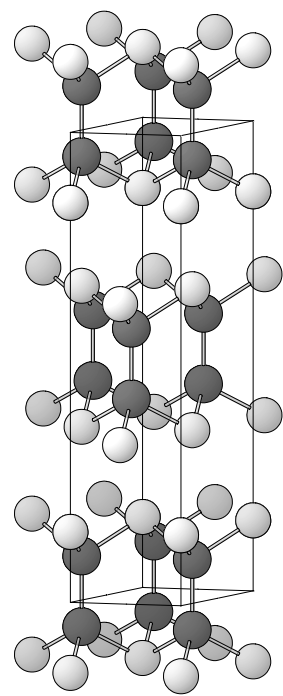


Fig. IV.12. **GaSe 2H**
Arrangement of Ga (dark) and Se (light) atoms.

Schubert K. et al. (1955) [1]

GaSe
 $a = 0.37425$, $c = 1.59191$ nm, $c/a = 4.254$, $V = 0.1931$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Se1	2 <i>i</i>	3 <i>m</i> .	$\frac{2}{3}$	$\frac{1}{3}$	0.150		non-coplanar triangle Ga ₃
Ga2	2 <i>h</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.425		tetrahedron GaSe ₃
Ga3	2 <i>g</i>	3 <i>m</i> .	0	0	0.075		tetrahedron GaSe ₃
Se4	2 <i>g</i>	3 <i>m</i> .	0	0	0.350		non-coplanar triangle Ga ₃

Transformation from published data (*P-6*): origin shift $\frac{2}{3} \frac{1}{3} \frac{1}{2}$
Experimental: single crystal, rotation photographs, X-rays

Remarks: Dominating modification in Se-poor samples. The same data are reported in [2]. The description in space group (174) *P-6* in [1] does not take into consideration all symmetry elements of the proposed structure (see [3]).
References: [1] Schubert K., Dörre E., Kluge M. (1955), *Z. Metallkd.* 46, 216-224. [2] Schubert K., Dörre E. (1953), *Naturwissenschaften* 40, 604-605. [3] Cenxual K., Gelato L.M., Penzo M., Parthé E. (1991), *Acta Crystallogr. B* 47, 433-439.