

Cs₂Na₆(Ga_{0.5}Ge_{0.5})₁₂GeO₂₄[OH]₆

hP52

(186) *P6₃mc* – d²c⁴ba**Cs₂Na₆Ga₆Ge₆O₂₄·Ge(OH)₆** [1], zeolite CAN(Ga,Ge)-OH

Structural features: (Ga,Ge)O₄ tetrahedra share vertices to form a CAN-type zeolite framework with channels delimited by 12-rings perpendicular to [001]; Cs at the centers of cancrinite-type cages (11-face polyhedra formed by six 4-rings, two planar and three non-planar 6-rings), Ge(OH)₆ octahedra in the channels (partial disorder), Na above non-planar 6-rings.

Lee Y. et al. (2000) [1]

Cs₂Ga₆Ge₇H₆Na₆O₃₀*a* = 1.295, *c* = 0.5117 nm, *c/a* = 0.395, *V* = 0.7432 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.3805	0.052	0.4305		non-colinear Ga ₂
M2	12 <i>d</i>	1	0.4193	0.084	0.094		tetrahedron O ₄
Na3	6 <i>c</i>	. <i>m</i> .	0.1361	0.8639	0.0957		tetrahedron O ₃ (OH)
O4	6 <i>c</i>	. <i>m</i> .	0.1873	0.8127	0.4932		non-colinear Ga ₂
O5	6 <i>c</i>	. <i>m</i> .	0.5746	0.4254	0.0368		non-colinear Ga ₂
(OH)6	6 <i>c</i>	. <i>m</i> .	0.9334	0.0667	0.24		non-colinear Ge ₂
Cs7	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.0881		non-coplanar triangle O ₃
Ge8	2 <i>a</i>	3 <i>m</i> .	0	0	0.0	0.5	octahedron (OH) ₆

M2 = 0.5Ga + 0.5Ge

Transformation from published data: origin shift 0 0 0.156

Experimental: single crystal, diffractometer, X-rays, synchrotron, R = 0.059, T = 293 K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Lee Y., Parise J.B., Tripathi A., Kim S.J., Vogt T. (2000), Microporous Mesoporous Mater. 39, 445-455.