

**Ba<sub>9</sub>Ge<sub>23</sub>O<sub>53</sub>[OH]<sub>4</sub>***hP*178(185) *P6<sub>3</sub>cm* – d<sup>8</sup>c<sup>12</sup>b<sup>2</sup>a**Ba<sub>9</sub>Ge<sub>23</sub>O<sub>53</sub>(OH)<sub>4</sub>** [1]

Structural features: GeO<sub>4</sub> tetrahedra, GeO<sub>5</sub> square pyramids, GeO<sub>6</sub> and Ge(O<sub>5</sub>[OH]) octahedra share vertices to form a 3D-framework with Ge<sub>3</sub>O<sub>10</sub> and Ge<sub>3</sub>(O,OH)<sub>11</sub> rings.

Ozima M. (1986) [1]

Ba<sub>9</sub>Ge<sub>23</sub>H<sub>4</sub>O<sub>57</sub>*a* = 1.16784, *c* = 1.92545 nm, *c/a* = 1.649, *V* = 2.2742 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.12179	0.34416	0.38585		non-colinear Ge <sub>2</sub>
O2	12 <i>d</i>	1	0.13759	0.3401	0.14328		non-colinear Ge <sub>2</sub>
Ge3	12 <i>d</i>	1	0.15277	0.49014	0.34992		tetrahedron O <sub>4</sub>
Ge4	12 <i>d</i>	1	0.15488	0.48501	0.10705		tetrahedron O <sub>4</sub>
O5	12 <i>d</i>	1	0.18179	0.59509	0.42248		non-colinear Ge <sub>2</sub>
O6	12 <i>d</i>	1	0.18431	0.60748	0.16816		non-colinear Ge <sub>2</sub>
O7	12 <i>d</i>	1	0.25243	0.51114	0.03396		non-colinear Ge <sub>2</sub>
O8	12 <i>d</i>	1	0.26211	0.51569	0.28506		non-colinear Ge <sub>2</sub>
O9	6 <i>c</i>	.. <i>m</i>	0.13133	0	0.67024		non-colinear Ge <sub>2</sub>
O10	6 <i>c</i>	.. <i>m</i>	0.13261	0	0.44998		non-colinear Ge <sub>2</sub>
M11	6 <i>c</i>	.. <i>m</i>	0.14188	0	0.8366		non-colinear Ge <sub>2</sub>
O12	6 <i>c</i>	.. <i>m</i>	0.14217	0	0.05265		non-colinear Ge <sub>2</sub>
Ge13	6 <i>c</i>	.. <i>m</i>	0.16165	0	0.14466		octahedron O <sub>5</sub> (OH)
Ge14	6 <i>c</i>	.. <i>m</i>	0.16615	0	0.35601		octahedron O <sub>5</sub> (OH)
(OH)15	6 <i>c</i>	.. <i>m</i>	0.2197	0	0.26259		single atom Ge
Ba16	6 <i>c</i>	.. <i>m</i>	0.30233	0	0.53016		10-vertex polyhedron O <sub>10</sub>
O17	6 <i>c</i>	.. <i>m</i>	0.45024	0	0.07014		non-colinear Ge <sub>2</sub>
O18	6 <i>c</i>	.. <i>m</i>	0.46266	0	0.31618		non-colinear Ge <sub>2</sub>
Ba19	6 <i>c</i>	.. <i>m</i>	0.67643	0	0.23732		9-vertex polyhedron O <sub>9</sub>
Ba20	6 <i>c</i>	.. <i>m</i>	0.68839	0	0.44781		pseudo Frank-Kasper O <sub>11</sub>
Ge21	4 <i>b</i>	3.. <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.22607		octahedron O <sub>6</sub>
Ge22	4 <i>b</i>	3.. <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.47635		octahedron O <sub>6</sub>
Ge23	2 <i>a</i>	3.. <i>m</i>	0	0	0.0		octahedron O <sub>6</sub>

M11 = 0.667O + 0.333OH

Experimental: single crystal, diffractometer, X-rays, R = 0.034, T = 300 K

Remarks: High-pressure phase; identical to the phase called Ba<sub>2</sub>Ge<sub>5</sub>O<sub>12</sub> in [2]. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Ozima M. (1986), Z. Kristallogr. 175, 125-130. [2] Ozima M., Susaki J.I., Akimoto S.I., Shimizu Y. (1982), J. Solid State Chem. 44, 307-317.