

**Mg<sub>3</sub>BeAl<sub>8</sub>O<sub>16</sub>***hP56*(186) *P6<sub>3</sub>mc* – c<sup>6</sup>b<sup>7</sup>a<sup>3</sup>**Mg<sub>3</sub>BeAl<sub>8</sub>O<sub>16</sub>** [2], taaffeite

Structural features: Close-packed O layers in hc<sub>3</sub> stacking; Al and Mg in octahedral and tetrahedral, Be in tetrahedral voids. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra share atoms with MgO<sub>6</sub> and additional AlO<sub>6</sub> octahedra, MgO<sub>4</sub> and BeO<sub>4</sub> tetrahedra to form a 3D-framework with spinel-type slabs.

Nuber B., Schmetzer K. (1983) [1]

Al<sub>8</sub>BeMg<sub>3</sub>O<sub>16</sub>*a* = 0.56867, *c* = 1.8337 nm, *c/a* = 3.225, *V* = 0.5135 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Al1	6 <i>c</i>	. <i>m</i> .	0.1665	0.8335	0.4475		octahedron O <sub>6</sub>
O2	6 <i>c</i>	. <i>m</i> .	0.185	0.8149	0.2608		tetrahedron BeAl <sub>2</sub> Mg
Al3	6 <i>c</i>	. <i>m</i> .	0.4987	0.5012	0.2018		octahedron O <sub>6</sub>
O4	6 <i>c</i>	. <i>m</i> .	0.5178	0.4822	0.0091		tetrahedron Al <sub>3</sub> Mg
O5	6 <i>c</i>	. <i>m</i> .	0.8146	0.1853	0.1424		tetrahedron Al <sub>3</sub> Mg
O6	6 <i>c</i>	. <i>m</i> .	0.8378	0.1622	0.3908		tetrahedron Al <sub>3</sub> Mg
Mg7	2 <i>b</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0417		tetrahedron O <sub>4</sub>
O8	2 <i>b</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1458		tetrahedron MgAl <sub>3</sub>
Be9	2 <i>b</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.3041		tetrahedron O <sub>4</sub>
O10	2 <i>b</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.3931		tetrahedron BeAl <sub>3</sub>
Al11	2 <i>b</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5758		octahedron O <sub>6</sub>
O12	2 <i>b</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.7604		tetrahedron Al <sub>4</sub>
Al13	2 <i>b</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.8577		tetrahedron O <sub>4</sub>
O14	2 <i>a</i>	3 <i>m</i> .	0	0	0.0		tetrahedron Al <sub>3</sub> Mg
Mg15	2 <i>a</i>	3 <i>m</i> .	0	0	0.1074		tetrahedron O <sub>4</sub>
Mg16	2 <i>a</i>	3 <i>m</i> .	0	0	0.3083		octahedron O <sub>6</sub>

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.6917Experimental: single crystal, diffractometer, X-rays, *wR* = 0.031

Remarks: Natural specimen from Niriella Village, Ratna Pura, Sri Lanka. Composition Mg<sub>2.81</sub>Fe<sub>0.15</sub>Zn<sub>0.04</sub>[BeAl<sub>8</sub>O<sub>16</sub>] from electron microprobe analysis. The authors state that Fe probably substitutes for Mg on tetrahedral sites. In table 2 of [1] the Wyckoff positions of former O3, O5 and O7 are misprinted as 2*a* instead of 2*b*.

References: [1] Nuber B., Schmetzer K. (1983), Neues Jahrb. Mineral., Monatsh. 1983, 393-402. [2] Peng C.C., Wang K.J. (1963), Sci. Sin. (Engl. Ed.) 12, 276-278.