

Li<sub>14</sub>(Be<sub>0.83</sub>B<sub>0.17</sub>)<sub>6</sub>[BO<sub>3</sub>]<sub>9</sub>

hP112

(176)  $P6_3/m - i^7h^2f^2edc$ **Li<sub>14</sub>Be<sub>5</sub>B(BO<sub>3</sub>)<sub>9</sub>** [1]

Structural features: (Be,B)O<sub>4</sub> tetrahedra and BO<sub>3</sub> trigonal units share vertices to form infinite slabs; Li in tetrahedral, trigonal and trigonal prismatic voids in and between the slabs, forming a 3D-framework with the polyhedra mentioned above.

Luce J.L. et al. (1994) [1]

B<sub>10</sub>Be<sub>5</sub>Li<sub>14</sub>O<sub>27</sub> $a = 0.773$ ,  $c = 1.8853$  nm,  $c/a = 2.439$ ,  $V = 0.9756$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12i	1	0.0888	0.2042	0.0929		non-colinear BBe
O2	12i	1	0.1279	0.5594	0.10726		non-colinear BBe
Li3	12i	1	0.3025	0.3268	0.1706		tetrahedron O <sub>4</sub>
Li4	12i	1	0.3235	0.3504	0.0361		tetrahedron O <sub>4</sub>
M5	12i	1	0.3477	0.0234	0.1115		tetrahedron O <sub>4</sub>
O6	12i	1	0.3931	0.1313	0.18812		non-colinear BBe
O7	12i	1	0.4645	0.1984	0.05063		non-colinear BBe
O8	6h	<i>m</i> ..	0.1823	0.3806	<sup>1</sup> / <sub>4</sub>		single atom B
B9	6h	<i>m</i> ..	0.3209	0.0198	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle O <sub>3</sub>
B10	4f	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1072		coplanar triangle O <sub>3</sub>
B11	4f	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5523		non-coplanar triangle O <sub>3</sub>
B12	4e	3..	0	0	0.0926		coplanar triangle O <sub>3</sub>
Li13	2d	-6..	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		trigonal prism O <sub>6</sub>
Li14	2c	-6..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		coplanar triangle O <sub>3</sub>

M5 = 0.833Be + 0.167B

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.048, T = 296 K

Remarks: In table 2 of [1] the *z*-coordinate of former Li3 is misprinted as 0.05361 instead of 0.5361 (checked on interatomic distances).

References: [1] Luce J.L., Schaffers K.I., Keszler D.A. (1994), Inorg. Chem. 33, 2453-2455.