

$(\text{Li}_{0.325}\text{Mg}_{0.675})_4\text{Ba}_3\text{Mg}_6\text{Ge}_6\text{O}_{0.32}$  $hP40$  $(176) P6_3/m - h^6cb$ **Li<sub>2.6</sub>Ba<sub>6</sub>Mg<sub>17.4</sub>Ge<sub>12</sub>O<sub>0.64</sub> [1]**

Structural features: Infinite columns of base-linked  $\text{Ge}(\text{Ba}_2\text{Mg}_4)\text{Mg}_3$  and  $\text{Ge}(\text{Ba}_4\text{Mg}_2)\text{Mg}_3$  tricapped trigonal prisms (partial substitution of Li for Mg ignored) share atoms to form a 3D-framework with  $\text{AlB}_2$ -type columns (7 prisms in the dented triangular cross-section); O in channels of hexagonal cross-section parallel to  $[001]$  (partial disorder).

Zürcher F., Nesper R. (2002) [1]

 $\text{Ba}_3\text{Ge}_6\text{Li}_{1.30}\text{Mg}_{8.70}\text{O}_{0.32}$  $a = 1.5378$ ,  $c = 0.4546$  nm,  $c/a = 0.296$ ,  $V = 0.9310$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ge1	6 <i>h</i>	<i>m</i> ..	0.04565	0.27467	$\frac{1}{4}$		monocapped trigonal prism Mg <sub>7</sub>
Ge2	6 <i>h</i>	<i>m</i> ..	0.13858	0.61439	$\frac{1}{4}$		square pyramid Mg <sub>5</sub>
M3	6 <i>h</i>	<i>m</i> ..	0.181	0.0999	$\frac{1}{4}$		6-vertex polyhedron O <sub>2</sub> Ge <sub>3</sub> Mg
Mg4	6 <i>h</i>	<i>m</i> ..	0.2466	0.3209	$\frac{1}{4}$		cuboctahedron Ge <sub>4</sub> Mg <sub>5</sub> Ba <sub>3</sub>
Mg5	6 <i>h</i>	<i>m</i> ..	0.4418	0.0253	$\frac{1}{4}$		cuboctahedron Ge <sub>4</sub> Mg <sub>4</sub> Ba <sub>4</sub>
Ba6	6 <i>h</i>	<i>m</i> ..	0.46674	0.28104	$\frac{1}{4}$		22-vertex polyhedron Ge <sub>8</sub> Mg <sub>10</sub> Ba <sub>4</sub>
M7	2 <i>c</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism Ge <sub>3</sub> Ba <sub>6</sub>
O8	2 <i>b</i>	-3..	0	0	0	0.32	square prism (cube) O <sub>2</sub> Mg <sub>6</sub>

 $\text{M3} = 0.65\text{Mg} + 0.35\text{Li}$ ;  $\text{M7} = 0.75\text{Mg} + 0.25\text{Li}$ Transformation from published data:  $y, x, -z$ Experimental: single crystal, diffractometer, X-rays,  $R = 0.028$ ,  $T = 298$  KReferences: [1] Zürcher F., Nesper R. (2002), *Z. Anorg. Allg. Chem.* 628, 1581-1589.