

$\text{Cu}_6\text{Bi}[\text{AsO}_4]_3[\text{OH}]_6[\text{H}_2\text{O}]_3$	<i>hP</i> 110	(176) $P6_3/m - i^6h^6d$
---	---------------	--------------------------

**BiCu<sub>6</sub>(AsO<sub>4</sub>)<sub>3</sub>(OH)<sub>6</sub>·3H<sub>2</sub>O** [1], mixite

Structural features: BiO<sub>6</sub>(OH)<sub>3</sub> tricapped trigonal prisms share vertices with AsO<sub>4</sub> tetrahedra to form infinite columns, which are interconnected via ribbons of edge-linked Cu(O<sub>2</sub>[OH]<sub>2</sub>) squares to form a 3D-framework; H<sub>2</sub>O in large channels parallel to [001] (partial disorder).

Miletich R. et al. (1997) [1]

As<sub>3</sub>BiCu<sub>6</sub>H<sub>12</sub>O<sub>21</sub>

$a = 1.3633$ ,  $c = 0.5913$  nm,  $c/a = 0.434$ ,  $V = 0.9517$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(OH <sub>2</sub> )1	12 <i>i</i>	1	0.077	0.19	0.112	0.083	
(OH <sub>2</sub> )2	12 <i>i</i>	1	0.117	0.185	0.012	0.167	
(OH <sub>2</sub> )3	12 <i>i</i>	1	0.175	0.161	0.007	0.083	
O4	12 <i>i</i>	1	0.1787	0.5742	0.0184		single atom As
(OH <sub>2</sub> )5	12 <i>i</i>	1	0.204	0.045	0.104	0.083	
Cu6	12 <i>i</i>	1	0.31429	0.41073	0.00284		square pyramid (OH) <sub>2</sub> O <sub>3</sub>
O7	6 <i>h</i>	<i>m</i> ..	0.0079	0.3987	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle AsCu <sub>2</sub>
(OH <sub>2</sub> )8	6 <i>h</i>	<i>m</i> ..	0.0179	0.0079	<sup>1</sup> / <sub>4</sub>	0.167	
As9	6 <i>h</i>	<i>m</i> ..	0.14974	0.49327	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>4</sub>
O10	6 <i>h</i>	<i>m</i> ..	0.2138	0.4147	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle AsCu <sub>2</sub>
(OH)11	6 <i>h</i>	<i>m</i> ..	0.3796	0.3699	<sup>1</sup> / <sub>4</sub>		non-colinear Cu <sub>2</sub>
(OH)12	6 <i>h</i>	<i>m</i> ..	0.4427	0.197	<sup>1</sup> / <sub>4</sub>		non-colinear Cu <sub>2</sub>
Bi13	2 <i>d</i>	-6..	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		tricapped trigonal prism O <sub>6</sub> (OH) <sub>3</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.042

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Miletich R., Zemmann J., Nowak M. (1997), Phys. Chem. Miner. 24, 411-422.