

LaBi[SCN]<sub>6</sub>[H<sub>2</sub>O]<sub>5</sub>*hP*54(176) *P*6<sub>3</sub>/*m* – i<sup>3</sup>hfd**b****Bi(SCN)<sub>6</sub>La(H<sub>2</sub>O)<sub>3</sub>·2H<sub>2</sub>O** [1]

Structural features: BiS<sub>6</sub> octahedra and LaN<sub>6</sub> trigonal prisms are interconnected via S=C=N linear units to form a 3D-framework; H<sub>2</sub>O in the layers containing the LaN<sub>6</sub> prisms (partial disorder).

Maniukiewicz W. et al. (1996) [1]

BiC<sub>6</sub>H<sub>10</sub>LaN<sub>6</sub>O<sub>5</sub>S<sub>6</sub>*a* = 0.82508, *c* = 1.8745 nm, *c/a* = 2.272, *V* = 1.1051 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	12 <i>i</i>	1	0.0066	0.3302	0.1195		non-colinear NS
S2	12 <i>i</i>	1	0.1824	0.3454	0.0715		single atom C
N3	12 <i>i</i>	1	0.4331	0.1074	0.1548		single atom C
(OH <sub>2</sub> )4	6 <i>h</i>	<i>m</i> ..	0.3501	0.3418	<sup>1</sup> / <sub>4</sub>		
(OH <sub>2</sub> )5	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.2161	0.5	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )6	4 <i>e</i>	3..	0	0	0.233	0.5	
La7	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 N <sub>6</sub> (OH <sub>2</sub> ) <sub>3</sub>
Bi8	2 <i>b</i>	-3..	0	0	0		octahedron S <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>Experimental: single crystal, diffractometer, X-rays, *R* = 0.028, *T* = 293 K

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] Maniukiewicz W., Sieron L., Bukowska Strzyzewska M., Turek A. (1996), *Acta Crystallogr. C* 52, 753-757.