

**Ba<sub>3</sub>SrNb<sub>2</sub>O<sub>9</sub>***hP30*(176) *P6<sub>3</sub>/m – ihf<sup>2</sup>ba***Ba<sub>3</sub>SrNb<sub>2</sub>O<sub>9</sub>** [1], perovskite 6H

Structural features: Close-packed BaO<sub>3</sub> layers in hc<sub>2</sub> stacking; Nb and Sr in octahedral (O<sub>6</sub>) voids. Pairs of face-linked NbO<sub>6</sub> octahedra (Nb<sub>2</sub> dumbbells) share vertices with single SrO<sub>6</sub> octahedra to form a 3D-framework.

Zandbergen H.W., Ijdo D.J.W. (1983) [1]

**Ba<sub>3</sub>Nb<sub>2</sub>O<sub>9</sub>Sr** $a = 0.60704$ ,  $c = 1.53758$  nm,  $c/a = 2.533$ ,  $V = 0.4907$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.2339	0.3554	0.0977		single atom Nb
O2	6 <i>h</i>	<i>m</i> ..	0.0424	0.4779	<sup>1</sup> / <sub>4</sub>		non-colinear Nb <sub>2</sub>
Nb3	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1535		octahedron O <sub>6</sub>
Ba4	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6185		octahedron O <sub>6</sub>
Sr5	2 <i>b</i>	-3..	0	0	0		octahedron O <sub>6</sub>
Ba6	2 <i>a</i>	-6..	0	0	<sup>1</sup> / <sub>4</sub>		anticuboctahedron O <sub>12</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>Experimental: powder, diffractometer, neutrons, R<sub>B</sub> = 0.023

References: [1] Zandbergen H.W., Ijdo D.J.W. (1983), Acta Crystallogr. C 39, 829-832.