

Ba₃NiSb₂O₉*hP30*(186) *P6₃mc* – *c*³*b*⁴*a*²**Ba₃NiSb₂O₉** [1], perovskite 6H

Structural features: Close-packed BaO₃ layers in hc₂ stacking; Ni and Sb in octahedral (O₆) voids. Units of two face-linked octahedra centered by Ni and Sb, respectively, share vertices with additional SbO₆ octahedra to form a 3D-framework. Substitution derivative of hexagonal BaTiO₃.

Köhl P., Reinen D. (1977) [1]

Ba₃NiO₉Sb₂*a* = 0.5837, *c* = 1.4392 nm, *c/a* = 2.466, *V* = 0.4246 nm³, *Z* = 2

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|------------|--------------|-----------------------------|-----------------------------|----------|------|-----------------------------------|
| O1 | 6 <i>c</i> | . <i>m</i> . | 0.16 | 0.84 | 0.3329 | | non-colinear SbNi |
| O2 | 6 <i>c</i> | . <i>m</i> . | 0.514 | 0.486 | 0.0009 | | non-colinear NiSb |
| O3 | 6 <i>c</i> | . <i>m</i> . | 0.835 | 0.165 | 0.1746 | | non-colinear Sb ₂ |
| Ba4 | 2 <i>b</i> | 3 <i>m</i> . | ¹ / ₃ | ² / ₃ | 0.15328 | | cuboctahedron O ₁₂ |
| Ni5 | 2 <i>b</i> | 3 <i>m</i> . | ¹ / ₃ | ² / ₃ | 0.4087 | | octahedron O ₆ |
| Sb6 | 2 <i>b</i> | 3 <i>m</i> . | ¹ / ₃ | ² / ₃ | 0.59482 | | octahedron O ₆ |
| Ba7 | 2 <i>b</i> | 3 <i>m</i> . | ¹ / ₃ | ² / ₃ | 0.84979 | | cuboctahedron O ₁₂ |
| Ba8 | 2 <i>a</i> | 3 <i>m</i> . | 0 | 0 | 0.0 | | anticuboctahedron O ₁₂ |
| Sb9 | 2 <i>a</i> | 3 <i>m</i> . | 0 | 0 | 0.2517 | | octahedron O ₆ |

Transformation from published data: origin shift 0 0 0.2465

Experimental: single crystal, diffractometer, X-rays, R = 0.030

References: [1] Köhl P., Reinen D. (1977), Z. Anorg. Allg. Chem. 433, 81-93.