

**Sm<sub>25</sub>Ni<sub>49</sub>P<sub>33</sub>** [1]

Structural features: Infinite columns of base-linked PSm<sub>6</sub>Ni<sub>3</sub>, P(Sm<sub>4</sub>Ni<sub>2</sub>)Ni<sub>3</sub>, P(Sm<sub>2</sub>Ni<sub>4</sub>)Ni<sub>3</sub> and NiSm<sub>6</sub>Ni<sub>3</sub> tricapped trigonal prisms share atoms to form a 3D-framework with two kinds of AlB<sub>2</sub>-type column (21 and 28 columns in the dented triangular cross-section, respectively); infinite columns of hexagonal cross-section parallel to [001].

Chykhrii S.I. et al. (2001) [1]

Ni<sub>49</sub>P<sub>33</sub>Sm<sub>25</sub>

*a* = 2.2096, *c* = 0.38734 nm, *c/a* = 0.175, *V* = 1.6378 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
P1	6 <i>m</i>	<i>m</i> ..	0.04933	0.29867	1/2		square pyramid Ni <sub>5</sub>
Ni2	6 <i>m</i>	<i>m</i> ..	0.12633	0.41367	1/2		non-colinear P <sub>2</sub>
Ni3	6 <i>m</i>	<i>m</i> ..	0.29233	0.06067	1/2		tetrahedron P <sub>4</sub>
Sm4	6 <i>m</i>	<i>m</i> ..	0.42613	0.03497	1/2		21-vertex polyhedron P <sub>7</sub> Ni <sub>8</sub> Sm <sub>6</sub>
Sm5	6 <i>l</i>	<i>m</i> ..	0.00073	0.18237	0		21-vertex polyhedron Ni <sub>8</sub> P <sub>7</sub> Sm <sub>6</sub>
Ni6	6 <i>l</i>	<i>m</i> ..	0.01933	0.32567	0		tetrahedron P <sub>4</sub>
P7	6 <i>l</i>	<i>m</i> ..	0.07333	0.44567	0		coplanar triangle Ni <sub>3</sub>
Ni8	6 <i>l</i>	<i>m</i> ..	0.18733	0.50567	0		cuboctahedron P <sub>3</sub> Ni <sub>6</sub> Sm <sub>3</sub>
P9	6 <i>l</i>	<i>m</i> ..	0.37233	0.09567	0		square pyramid Ni <sub>5</sub>
Ni10	6 <i>l</i>	<i>m</i> ..	0.48933	0.15067	0		tricapped trigonal prism P <sub>3</sub> Sm <sub>6</sub>
P11	3 <i>k</i>	<i>mm</i> 2	0.05433	0.94567	1/2		coplanar triangle Ni <sub>3</sub>
Ni12	3 <i>k</i>	<i>mm</i> 2	0.11833	0.88167	1/2		tricapped trigonal prism P <sub>3</sub> Sm <sub>6</sub>
P13	3 <i>k</i>	<i>mm</i> 2	0.23833	0.76167	1/2		coplanar triangle Ni <sub>3</sub>
Ni14	3 <i>k</i>	<i>mm</i> 2	0.29373	0.70627	1/2		11-vertex polyhedron PNi <sub>10</sub>
Sm15	3 <i>k</i>	<i>mm</i> 2	0.43233	0.56767	1/2		22-vertex polyhedron Ni <sub>12</sub> P <sub>6</sub> Sm <sub>4</sub>
Sm16	3 <i>k</i>	<i>mm</i> 2	0.60733	0.39267	1/2		pseudo Frank-Kasper P <sub>6</sub> Ni <sub>6</sub> Sm <sub>8</sub>
Sm17	3 <i>k</i>	<i>mm</i> 2	0.78553	0.21447	1/2		21-vertex polyhedron Ni <sub>8</sub> P <sub>7</sub> Sm <sub>6</sub>
P18	3 <i>k</i>	<i>mm</i> 2	0.88233	0.11767	1/2		coplanar triangle Ni <sub>3</sub>
Ni19	3 <i>k</i>	<i>mm</i> 2	0.93833	0.06167	1/2		coplanar triangle P <sub>3</sub>
Sm20	3 <i>j</i>	<i>mm</i> 2	0.18003	0.81997	0		22-vertex polyhedron Ni <sub>10</sub> P <sub>8</sub> Sm <sub>4</sub>
Ni21	3 <i>j</i>	<i>mm</i> 2	0.36933	0.63067	0		square prism (cube) Ni <sub>8</sub>
Ni22	3 <i>j</i>	<i>mm</i> 2	0.49033	0.50967	0		coplanar triangle P <sub>3</sub>
P23	3 <i>j</i>	<i>mm</i> 2	0.55333	0.44667	0		coplanar triangle Ni <sub>3</sub>
P24	3 <i>j</i>	<i>mm</i> 2	0.72133	0.27867	0		coplanar triangle Ni <sub>3</sub>
Ni25	3 <i>j</i>	<i>mm</i> 2	0.83833	0.16167	0		10-vertex polyhedron P <sub>4</sub> Ni <sub>4</sub> Sm <sub>2</sub>
Ni26	1 <i>e</i>	-6 <i>m</i> 2	2/3	1/3	0		coplanar triangle P <sub>3</sub>
Sm27	1 <i>a</i>	-6 <i>m</i> 2	0	0	0		pseudo Frank-Kasper P <sub>6</sub> Ni <sub>6</sub> Sm <sub>8</sub>

Transformation from published data: -*x*, -*y*, -*z*; origin shift 2/3 1/3 0

Experimental: powder, diffractometer, X-rays, R<sub>p</sub> = 0.180

References: [1] Chykhrii S.I., Babizhets'kii V.S., Kuz'ma Y.B. (2001), *Z. Anorg. Allg. Chem.* 627, 1319-1324.