

Ba₈Ta₆NiO₂₄*hP*118(185) $P6_3cm - d^4c^9b^3a^2$ **Ba₈Ta₆NiO₂₄** [1]

Structural features: Close-packed BaO₃ layers in (hc₃)₂ stacking; Ta and Ni in octahedral voids. Vacancy derivative of perovskite 8H, A₈[B₆B'□]O₂₄.

Abakumov A.M. et al. (1996) [1]

Ba₈NiO₂₄Ta₆ $a = 1.00746$, $c = 1.90122$ nm, $c/a = 1.887$, $V = 1.6712$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.168	0.334	0.008		non-colinear Ta ₂
O2	12 <i>d</i>	1	0.17	0.49	0.386		non-colinear Ta ₂
O3	12 <i>d</i>	1	0.174	0.486	0.126		non-colinear TaNi
O4	12 <i>d</i>	1	0.347	0.506	0.253		non-colinear NiTa
O5	6 <i>c</i>	.. <i>m</i>	0.145	0	0.754		single atom Ta
O6	6 <i>c</i>	.. <i>m</i>	0.156	0	0.129		non-colinear Ta ₂
O7	6 <i>c</i>	.. <i>m</i>	0.19	0	0.379		single atom Ta
Ta8	6 <i>c</i>	.. <i>m</i>	0.3321	0	0.072		octahedron O ₆
Ba9	6 <i>c</i>	.. <i>m</i>	0.334	0	0.26		anticuboctahedron O ₁₂
Ta10	6 <i>c</i>	.. <i>m</i>	0.3413	0	0.447		octahedron O ₆
O11	6 <i>c</i>	.. <i>m</i>	0.499	0	0.012		non-colinear Ta ₂
Ba12	6 <i>c</i>	.. <i>m</i>	0.658	0	0.147		cuboctahedron O ₁₂
Ba13	6 <i>c</i>	.. <i>m</i>	0.6913	0	0.37		cuboctahedron O ₁₂
Ba14	4 <i>b</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0155		cuboctahedron O ₁₂
M15	4 <i>b</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.193	0.9	octahedron O ₆
Ta16	4 <i>b</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.326	0.85	octahedron O ₆
Ba17	2 <i>a</i>	3.. <i>m</i>	0	0	0.0		cuboctahedron O ₁₂
Ta18	2 <i>a</i>	3.. <i>m</i>	0	0	0.199		octahedron O ₆

M15 = 0.83Ni + 0.17Ta

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.75

Experimental: powder, diffractometer, X-rays, R = 0.028

References: [1] Abakumov A.M., Van Tendeloo G., Scheglov A.A., Shpanchenko R.V., Antipov E.V. (1996), J. Solid State Chem. 125, 102-107.