

Ba ₃ HoRhAlO _{7.5}	<i>hP30</i>	(187) <i>P-6m2</i> – n ² kji ² h ² gba
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Ba₆Ho₂Rh₂Al₂O₁₅ [1], perovskite 6H; Ba₆Rh₄Al₂O₁₅ [2]

Structural features: Close-packed BaO₃ layers (partial vacancies ignored) in hc₂ stacking; Ho, Rh and Al in octahedral (O₆) voids (Al displaced from the octahedron centers). Substitution derivative of hexagonal BaTiO₃ (perovskite 6H), A₃[BB'B'']O_{9-x}.

Schlüter D., Müller Buschbaum H. (1993) [1]

AlBa₃HoO_{7.50}Rh

a = 0.58718, *c* = 1.46939 nm, *c/a* = 2.502, *V* = 0.4387 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>n</i>	. <i>m</i> .	0.1825	0.8175	0.325		non-colinear AlHo
O2	6 <i>n</i>	. <i>m</i> .	0.8355	0.1645	0.162		non-colinear RhHo
O3	3 <i>k</i>	<i>mm2</i>	0.46	0.54	1/2	0.33	4-vertex polyhedron O ₂ Al ₂
O4	3 <i>j</i>	<i>mm2</i>	0.511	0.489	0	0.67	non-colinear Rh ₂
Rh5	2 <i>i</i>	3 <i>m</i> .	2/3	1/3	0.0872		octahedron O ₆
Ba6	2 <i>i</i>	3 <i>m</i> .	2/3	1/3	0.3212		9-vertex polyhedron O ₉
Ba7	2 <i>h</i>	3 <i>m</i> .	1/3	2/3	0.1484		cuboctahedron O ₁₂
Al8	2 <i>h</i>	3 <i>m</i> .	1/3	2/3	0.3746		octahedron O ₆
Ho9	2 <i>g</i>	3 <i>m</i> .	0	0	0.2508		octahedron O ₆
Ba10	1 <i>b</i>	-6 <i>m2</i>	0	0	1/2		anticuboctahedron O ₁₂
Ba11	1 <i>a</i>	-6 <i>m2</i>	0	0	0		anticuboctahedron O ₁₂

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.046

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. A partly ordered atom arrangement is reported for Ba₆Rh₄Al₂O₁₅ in [2], Ba₆(Al,Rh)₂Rh₂(Rh,Al)₂O₁₅.

References: [1] Schlüter D., Müller Buschbaum H. (1993), J. Alloys Compd. 191, 305-308. [2] Schlüter D., Müller Buschbaum H. (1993), J. Alloys Compd. 197, 51-55.