

Ba₅Re₃BrO₁₅*hP48*(185) *P6₃cm – d²c³ba***Ba₅(ReO₅)₃Br** [1]

Structural features: Infinite columns of face-linked BrBa₆ octahedra parallel to [001]; single ReO₅ square pyramids and additional Ba between the columns.

Baud G. et al. (1979) [1]

Ba₅BrO₁₅Re₃ $a = 1.0967$, $c = 0.779$ nm, $c/a = 0.710$, $V = 0.8114$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.1313	0.5812	0.2046		single atom Re
O2	12 <i>d</i>	1	0.1324	0.389	0.0312		single atom Re
O3	6 <i>c</i>	.. <i>m</i>	0.2959	0	0.349		single atom Re
Re4	6 <i>c</i>	.. <i>m</i>	0.3924	0	0.1806		square pyramid O ₅
Ba5	6 <i>c</i>	.. <i>m</i>	0.7347	0	0.2295		pseudo Frank-Kasper O ₉ Br ₂
Ba6	4 <i>b</i>	3.. <i></i>	¹ / ₃	² / ₃	0.4697		tricapped trigonal prism O ₉
Br7	2 <i>a</i>	3.. <i>m</i>	0	0	0.0		9-vertex polyhedron Ba ₆ O ₃

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.0298

Experimental: single crystal, diffractometer, X-rays, R = 0.034

References: [1] Baud G., Besse J.P., Sueur G., Chevalier R. (1979), Mater. Res. Bull. 14, 675-682.