

Ba ₅ Re ₃ ClO ₁₅	<i>hP50</i>	(185) <i>P6₃cm</i> – d ² c ³ ba ²
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Ba₅(ReO₅)₃Cl [1]

Structural features: Infinite columns of face-linked ClBa₆ octahedra (split Cl site) parallel to [001]; single ReO₅ square pyramids and additional Ba between the columns.

Besse J.P. et al. (1979) [1]

Ba₅ClO₁₅Re₃

a = 1.0935, *c* = 0.7795 nm, *c/a* = 0.713, *V* = 0.8072 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.129	0.577	0.316		single atom Re
O2	12 <i>d</i>	1	0.258	0.39	0.017		single atom Re
O3	6 <i>c</i>	.. <i>m</i>	0.298	0	0.166		single atom Re
Re4	6 <i>c</i>	.. <i>m</i>	0.3919	0	0.3445		square pyramid O ₅
Ba5	6 <i>c</i>	.. <i>m</i>	0.7382	0	0.2955		pseudo Frank-Kasper O ₉ Cl ₂
Ba6	4 <i>b</i>	3..	¹ / ₃	² / ₃	0.057		tricapped trigonal prism O ₉
Cl7	2 <i>a</i>	3.. <i>m</i>	0	0	0.0	0.5	single atom Cl
Cl8	2 <i>a</i>	3.. <i>m</i>	0	0	0.133	0.5	single atom Cl

Transformation from published data: origin shift 0 0 0.943

Experimental: single crystal, diffractometer, X-rays, R = 0.068

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Besse J.P., Baud G., Levasseur G., Chevalier R. (1979), Acta Crystallogr. B 35, 1756-1759.