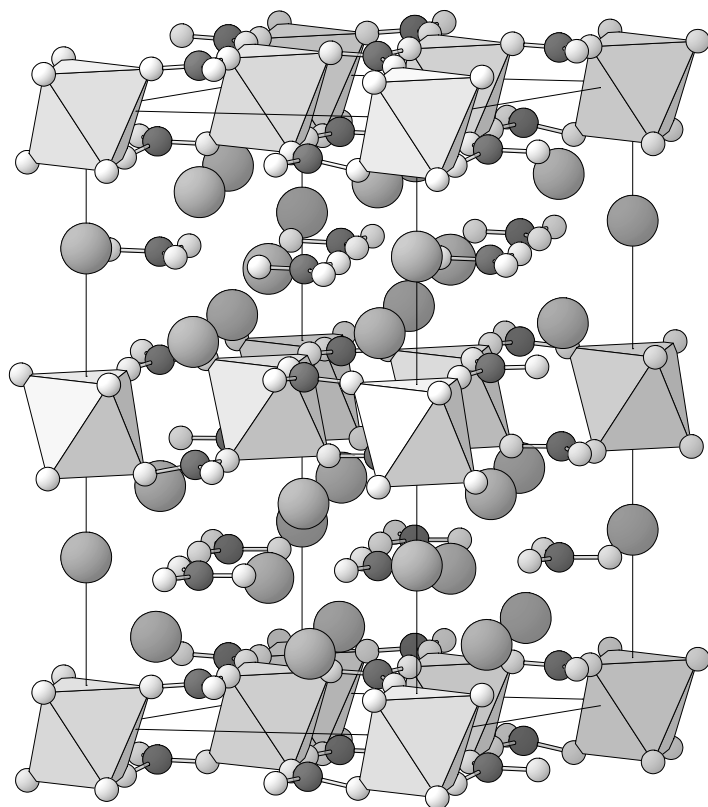


LuBa₃(BO₃)₃ [1]; Ba₃Ho(BO₃)₃ [1]

Structural features: LuO₆ octahedra share vertices with BO₃ trigonal units (perpendicular to [001]) to form infinite slabs; Ba and additional BO₃ units between the slabs. See Fig. IV.33.

Fig. IV.33. **LuBa₃(BO₃)₃**

Arrangement of LuO₆ octahedra, BO₃ triangles (B atoms dark, O atoms light) and Ba atoms (large).

Ilyukhin A.B., Dzhurinskii B.F. (1993) [1]

B₃Ba₃LuO₉

$a = 0.9382$, $c = 1.7421$ nm, $c/a = 1.857$, $V = 1.3280$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>d</i>	1	0.144	0.48	0.0798		single atom B
O2	12 <i>d</i>	1	0.149	0.334	0.2528		single atom B
O3	12 <i>d</i>	1	0.153	0.48	0.4283		single atom B
O4	6 <i>c</i>	.. <i>m</i>	0.178	0	0.413		single atom B
O5	6 <i>c</i>	.. <i>m</i>	0.197	0	0.069		single atom B
B6	6 <i>c</i>	.. <i>m</i>	0.33	0	0.43		non-coplanar triangle O ₃
B7	6 <i>c</i>	.. <i>m</i>	0.34	0	0.251		non-coplanar triangle O ₃
B8	6 <i>c</i>	.. <i>m</i>	0.341	0	0.076		coplanar triangle O ₃
O9	6 <i>c</i>	.. <i>m</i>	0.477	0	0.2527		single atom B
Ba10	6 <i>c</i>	.. <i>m</i>	0.6572	0	0.3715		9-vertex polyhedron O ₉
Ba11	6 <i>c</i>	.. <i>m</i>	0.6766	0	0.1289		9-vertex polyhedron O ₉
Lu12	4 <i>b</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0042		octahedron O ₆
Ba13	4 <i>b</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.2278		non-coplanar hexagon O ₆
Lu14	2 <i>a</i>	3.. <i>m</i>	0	0	0.0		octahedron O ₆
Ba15	2 <i>a</i>	3.. <i>m</i>	0	0	0.2759		9-vertex polyhedron O ₉

Transformation from published data: $-x, -y, -z$

Experimental: single crystal, diffractometer, X-rays, $R = 0.043$

References: [1] Ilyukhin A.B., Dzhurinskii B.F. (1993), Russ. J. Inorg. Chem. 38, 1516-1520 (Zh. Neorg. Khim. 38, 1625-1630).