

BaSr_{0.5}Lu₁₁O₁₈*hP68*(176) *P6₃/m – h¹⁰fc***Ba₂SrLu₂₂O₃₆** [1]

Structural features: Double infinite chains of edge-linked LuO₆ octahedra and single infinite columns of base-linked LuO₆ trigonal prisms (partial vacancies ignored) share atoms to form a 3D-framework; Ba and Sr in channels parallel to [001] (partial disorder).

Krüger J., Müller Buschbaum H. (1985) [1]

BaLu₁₁O₁₈Sr_{0.50}*a* = 1.76, *c* = 0.333 nm, *c/a* = 0.189, *V* = 0.8933 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Lu1	6 <i>h</i>	<i>m</i> ..	0.0094	0.3397	1/4	0.667	monocapped trigonal prism O ₇
Lu2	6 <i>h</i>	<i>m</i> ..	0.1045	0.5536	1/4		octahedron O ₆
Lu3	6 <i>h</i>	<i>m</i> ..	0.1177	0.2309	1/4		octahedron O ₆
O4	6 <i>h</i>	<i>m</i> ..	0.16	0.017	1/4		non-coplanar triangle Lu ₃
O5	6 <i>h</i>	<i>m</i> ..	0.186	0.487	1/4		non-coplanar triangle Lu ₃
O6	6 <i>h</i>	<i>m</i> ..	0.25	0.358	1/4		square pyramid Lu ₅
O7	6 <i>h</i>	<i>m</i> ..	0.308	0.219	1/4		square pyramid Lu ₅
Lu8	6 <i>h</i>	<i>m</i> ..	0.4326	0.2122	1/4		octahedron O ₆
O9	6 <i>h</i>	<i>m</i> ..	0.536	0.181	1/4		non-coplanar triangle Lu ₃
O10	6 <i>h</i>	<i>m</i> ..	0.561	0.026	1/4		non-coplanar triangle Lu ₃
Sr11	4 <i>f</i>	3..	1/3	2/3	0.0	0.25	
Ba12	2 <i>c</i>	-6..	1/3	2/3	1/4	0.5	
Ba13	2 <i>b</i>	-3..	0	0	0	0.5	

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

Experimental: single crystal, diffractometer, X-rays, R = 0.100

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

References: [1] Krüger J., Müller Buschbaum H. (1985), Z. Anorg. Allg. Chem. 526, 60-66.