

La₈Ru₄O₂₁*hP66*(185) *P6₃cm – d²c⁶ba***La₈Ru₄O₂₁** [1]

Structural features: Ru₄O₂₁ units consisting of a central RuO₆ octahedron sharing vertices with three surrounding RuO₆ octahedra.

Cotton F.A., Rice C.E. (1978) [1]

La₈O₂₁Ru₄*a* = 0.9885, *c* = 1.0805 nm, *c/a* = 1.093, *V* = 0.9143 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.1634	0.4364	0.27		single atom Ru
O2	12 <i>d</i>	1	0.2981	0.4539	0.0348		single atom Ru
O3	6 <i>c</i>	.. <i>m</i>	0.1543	0	0.1081		single atom Ru
O4	6 <i>c</i>	.. <i>m</i>	0.1596	0	0.3854		non-colinear Ru ₂
La5	6 <i>c</i>	.. <i>m</i>	0.242	0	0.7321		9-vertex polyhedron O ₉
Ru6	6 <i>c</i>	.. <i>m</i>	0.3551	0	0.4017		octahedron O ₆
La7	6 <i>c</i>	.. <i>m</i>	0.3972	0	0.093		square antiprism O ₈
O8	6 <i>c</i>	.. <i>m</i>	0.5585	0	0.3754		single atom Ru
La9	4 <i>b</i>	3.. ₂	¹ / ₃	² / ₃	0.3831		icosahedron O ₉ Ru ₃
Ru10	2 <i>a</i>	3.. ₂	0	0	0.0		octahedron O ₆

Transformation from published data: origin shift 0 0 0.5

Experimental: single crystal, diffractometer, X-rays, R = 0.027

References: [1] Cotton F.A., Rice C.E. (1978), J. Solid State Chem. 24, 359-365.