

La₁₂Re₅C₁₅*hP32*(189) *P-62m* – $\text{kg}^2\text{f}^4\text{d}$ **La₁₂Re₅C₁₅** [1]

Structural features: Planar Re₃C₃(C₂)₃ units (a Re₃ triangle with one C above each edge and a C₂ dumbbell bonded to each Re) and single ReC₃ trigonal units. One C₂ dumbbell (0.128 nm) for three single C.

Pöttgen R. et al. (1994) [1]

C₁₅La₁₂Re₅ $a = 1.1168$, $c = 0.5453$ nm, $c/a = 0.488$, $V = 0.5890$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	6 <i>k</i>	<i>m</i> ..	0.286	0.469	$\frac{1}{2}$		single atom Re
La2	6 <i>j</i>	<i>m</i> ..	0.2716	0.4581	0		6-vertex polyhedron C ₆
La3	3 <i>g</i>	<i>m2m</i>	0.4181	0	$\frac{1}{2}$		bicapped square prism C ₈ Re ₂
La4	3 <i>g</i>	<i>m2m</i>	0.7956	0	$\frac{1}{2}$		tetrahedron C ₄
Re5	3 <i>f</i>	<i>m2m</i>	0.1518	0	0		coplanar triangle C ₃
C6	3 <i>f</i>	<i>m2m</i>	0.327	0	0		single atom C
C7	3 <i>f</i>	<i>m2m</i>	0.442	0	0		single atom C
C8	3 <i>f</i>	<i>m2m</i>	0.809	0	0		non-colinear Re ₂
Re9	2 <i>d</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		coplanar triangle C ₃

Experimental: single crystal, diffractometer, X-rays, wR = 0.035

Remarks: Refinement of the site occupancies showed no significant deviation from unity.

References: [1] Pöttgen R., Block G., Jeitschko W., Behrens R.K. (1994), Z. Naturforsch. B 49, 1081-1088.