$LaMo_2O_5$	*hP*96	(186) $P6_3mc$ – $d^2c^{10}b^5a$

$LaMo_2O_5$ [1]
Structural features: Mo_6O_{18} units (a Mo_6 octahedron surrounded by an O_{12} anticuboctahedron and a large O_6 octahedron) and infinite layers where Mo_3 triangular clusters are interconnected via slightly longer Mo-Mo distances.

Hibble S.J. et al. (1998) [1]
$LaMo_2O_5$
a = 0.837, c = 1.91484 nm, c/a = 2.288, V = 1.1618 nm^3, Z = 12

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*d*	1	0.015	0.342	0.247		non-colinear Mo_2
O2	12*d*	1	0.331	0.006	0.001		non-colinear Mo_2
O3	6*c*	.*m*.	0.104	0.896	0.377		non-coplanar triangle Mo_3
Mo4	6*c*	.*m*.	0.111	0.889	0.196		5-vertex polyhedron O_5
O5	6*c*	.*m*.	0.225	0.775	0.143		single atom Mo
Mo6	6*c*	.*m*.	0.231	0.769	0.435		octahedron O_6
O7	6*c*	.*m*.	0.444	0.556	0.368		non-coplanar triangle Mo_3
La8	6*c*	.*m*.	0.5203	0.4797	0.102		square pyramid O_5
Mo9	6*c*	.*m*.	0.562	0.438	0.431		octahedron O_6
O10	6*c*	.*m*.	0.776	0.224	0.36		non-coplanar triangle Mo_3
O11	6*c*	.*m*.	0.887	0.113	0.128		non-colinear Mo_2
Mo12	6*c*	.*m*.	0.892	0.108	0.312		5-vertex polyhedron O_5
O13	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.013		non-coplanar triangle Mo_3
La14	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.244		cuboctahedron O_{12}
O15	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.489		non-coplanar triangle Mo_3
O16	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.64		tetrahedron La_4
La17	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.758		10-vertex polyhedron O_{10}
La18	2*a*	3*m*.	0	0	0.0		anticuboctahedron O_{12}

Transformation from published data: origin shift 0 0 0.746
Experimental: powder, diffractometer, neutrons, time-of-flight, wR_p = 0.086, T = 300 K

Remarks: Model for local ordering; the average structure was refined in space group (194) $P6_3/mmc$.

References: [1] Hibble S.J., Cooper S.P., Hannon A.C., Patat S., McCarroll W.H. (1998), Inorg. Chem. 37, 6839-6846.