$LiBa_4Nb_3O_{12}$	*hP*40	(186) $P6_3mc$ – $c^4b^5a^3$

$Ba_8Nb_6Li_2O_{24}$ [1], perovskite 8H
Structural features: Close-packed BaO_3 layers in hc_3 stacking; Li and Nb in octahedral voids. Units of two face-linked octahedra (centered by Li and Nb, respectively) share vertices with additional NbO_6 octahedra to form a 3D-framework.

Negas T. et al. (1973) [1]
$Ba_4LiNb_3O_{12}$
$a = 0.58035$, $c = 1.9076$ nm, $c/a = 3.287$, $V = 0.5564$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	6*c*	.*m*.	0.16667	0.83333	0.125		colinear NbLi
O2	6*c*	.*m*.	0.16667	0.83333	0.375		colinear Nb_2
O3	6*c*	.*m*.	0.5	0.5	0.0		colinear Nb_2
O4	6*c*	.*m*.	0.83333	0.16667	0.25		non-colinear LiNb
Nb5	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0625		octahedron O_6
Ba6	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.25		anticuboctahedron O_{12}
Nb7	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.4375		octahedron O_6
Ba8	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.625		cuboctahedron O_{12}
Ba9	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.875		cuboctahedron O_{12}
Ba10	2*a*	3*m*.	0	0	0.0		cuboctahedron O_{12}
Li11	2*a*	3*m*.	0	0	0.1875		octahedron O_6
Nb12	2*a*	3*m*.	0	0	0.3125		octahedron O_6

Transformation from published data: origin shift 0 0 0.5
Experimental: powder, diffractometer, X-rays

Remarks: Idealized coordinates.

References: [1] Negas T., Roth R.S., Parker H.S., Brower W.S. (1973), J. Solid State Chem. 8, 1-13.