

NaBa ₃ La[PO ₄] ₃ F	<i>hP44</i>	(174) <i>P</i> -6 – <i>l</i> ² <i>k</i> ⁴ <i>j</i> ⁴ <i>ihg</i> ²
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Na₂Ba₆La₂(PO₄)₆F₂ [1], apatite family; Na_{6,9}Ca_{3,1}(SO₄)₆(OH)_{1,1} [2], cesanite

Structural features: Infinite columns of base-linked (La,Na)O₆O₃ and (Ba,Na)O₆O₃ tricapped trigonal prisms share atoms with PO₄ tetrahedra to form a 3D-framework; F in infinite columns of face-linked (Ba,Na)₆ and (Ba,La)₆ octahedra parallel to [001] (partial disorder).

Mathew M. et al. (1979) [1]

Ba₃FLaNaO₁₂P₃

a = 0.99392, *c* = 0.74419 nm, *c/a* = 0.749, *V* = 0.6367 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>l</i>	1	0.074	0.351	0.15		single atom P
O2	6 <i>l</i>	1	0.362	0.274	0.321		single atom P
M3	3 <i>k</i>	<i>m</i> ..	0.021	0.2545	¹ / ₂		monocapped trigonal prism O ₅ F ₂
O4	3 <i>k</i>	<i>m</i> ..	0.131	0.621	¹ / ₂		single atom P
P5	3 <i>k</i>	<i>m</i> ..	0.407	0.3815	¹ / ₂		tetrahedron O ₄
O6	3 <i>k</i>	<i>m</i> ..	0.536	0.126	¹ / ₂		single atom P
P7	3 <i>j</i>	<i>m</i> ..	0.0378	0.414	0		tetrahedron O ₄
O8	3 <i>j</i>	<i>m</i> ..	0.137	0.59	0		single atom P
M9	3 <i>j</i>	<i>m</i> ..	0.2551	0.2324	0		
O10	3 <i>j</i>	<i>m</i> ..	0.497	0.146	0		single atom P
M11	2 <i>i</i>	3..	² / ₃	¹ / ₃	0.2801		tricapped trigonal prism O ₉
M12	2 <i>h</i>	3..	¹ / ₃	² / ₃	0.2486		trigonal prism O ₆
F13	2 <i>g</i>	3..	0	0	0.037	0.5	
F14	2 <i>g</i>	3..	0	0	0.303	0.5	single atom F

M3 = 0.904Ba + 0.096Na; M9 = 0.667Ba + 0.333La; M11 = 0.500La + 0.500Na; M12 = 0.645Ba + 0.355Na

Transformation from published data: -*y*, -*x*, -*z*; origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.074

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

References: [1] Mathew M., Mayer I., Dickens B., Schroeder L.W. (1979), J. Solid State Chem. 28, 79-95. [2] Piotrowski A., Kahlenberg V., Fischer R.X., Lee Y., Parise J.B. (2002), Am. Mineral. 87, 715-720.