

Ba ₂ [P ₂ O ₇]	<i>hP39</i>	(189) <i>P-62m</i> – lkihgf ² e
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Ba₂P₂O₇ σ [1]

Structural features: Directly superposed hexagon-mesh Ba layers; units of two vertex-linked PO₄ octahedra (parallel to [001], splitting of the bridging O sites to assure an angle Si-O-Si < 180°) center the hexagons.

El Belghitti A.A. et al. (1995) [1]

Ba₂O_{6.99}P₂

a = 0.9415, *c* = 0.7078 nm, *c/a* = 0.752, *V* = 0.5434 nm³, *Z* = 3

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>l</i>	1	0.3232	0.5112	0.2212		single atom P
O2	6 <i>k</i>	<i>m</i> ..	0.254	0.628	¹ / ₂	0.33	
O3	6 <i>i</i>	.. <i>m</i>	0.1528	0	0.2686		single atom P
P4	4 <i>h</i>	3.. <i></i>	¹ / ₃	² / ₃	0.2835		
Ba5	3 <i>g</i>	<i>m2m</i>	0.7112	0	¹ / ₂		10-vertex polyhedron O ₁₀
O6	3 <i>f</i>	<i>m2m</i>	0.076	0	0	0.33	non-colinear O ₂
Ba7	3 <i>f</i>	<i>m2m</i>	0.3822	0	0		11-vertex polyhedron O ₁₁
P8	2 <i>e</i>	3. <i>m</i>	0	0	0.2129		trigonal prism O ₆

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

Experimental: single crystal, diffractometer, X-rays, *R* = 0.025, *T* = 298 K

Remarks: Phase stated to be stable at *T* > 1000 K, however, the sample was slowly cooled to rt. Short interatomic distances for partly occupied site(s).

References: [1] El Belghitti A.A., Elmarzouki A., Boukhari A., Holt E.M. (1995), Acta Crystallogr. C 51, 1478-1480.