

Cd₅[PO₄]₃Br*hP*60(176) *P*6₃/*m* – ih⁴fe⁴ba**Cd₅(PO₄)₃Br** [1], apatite family

Structural features: Infinite columns of base-linked CdO₆ trigonal prisms share vertices with PO₄ tetrahedra to form a 3D-framework; Br in infinite columns of face-linked Cd₆ octahedra (partial vacancies ignored) parallel to [001] (high degree of disorder).

Sudarsanan K. et al. (1977) [1]

Br_{0.82}Cd_{4.82}O₁₂P₃*a* = 0.9733, *c* = 0.6468 nm, *c/a* = 0.665, *V* = 0.5306 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.348	0.0784	0.0597		single atom P
O2	6 <i>h</i>	<i>m</i> ..	0.1495	0.5042	¹ / ₄		single atom P
Cd3	6 <i>h</i>	<i>m</i> ..	0.2764	0.2562	¹ / ₄	0.965	non-coplanar triangle O ₃
P4	6 <i>h</i>	<i>m</i> ..	0.4056	0.0277	¹ / ₄		tetrahedron O ₄
O5	6 <i>h</i>	<i>m</i> ..	0.5903	0.1334	¹ / ₄		single atom P
Cd6	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.0054	0.963	trigonal prism O ₆
Br7	4 <i>e</i>	3..	0	0	0.05	0.021	
Br8	4 <i>e</i>	3..	0	0	0.1	0.043	
Br9	4 <i>e</i>	3..	0	0	0.15	0.106	
Br10	4 <i>e</i>	3..	0	0	0.2	0.176	
Br11	2 <i>b</i>	-3..	0	0	0	0.007	
Br12	2 <i>a</i>	-6..	0	0	¹ / ₄	0.122	

Transformation from published data: *y*,*x*,*-z*Experimental: single crystal, diffractometer, X-rays, *R* = 0.040

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

References: [1] Sudarsanan K., Young R.A., Wilson A.J.C. (1977), Acta Crystallogr. B 33, 3136-3142.