

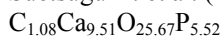
hP56

(174) $P-6 - I^4k^4j^4ihg^2$

Ca_{9.75}(PO₄)_{5.5}(CO₃)_{1.5} [1], apatite family

Structural features: Infinite columns of base-linked CaO₆O₃ tricapped trigonal prisms share atoms with PO₄ tetrahedra to form a 3D-framework (partial vacancies ignored); CO₃ trigonal units in infinite columns of face-linked Ca₆ octahedra parallel to [001] (units parallel to [001], partial orientational disorder).

Suetsugu Y. et al. (2000) [1]



$a = 0.948$, $c = 0.6898$ nm, $c/a = 0.728$, $V = 0.5369$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>l</i>	1	0.0276	0.1271	0.3411	0.18	non-colinear O ₂
O2	6 <i>l</i>	1	0.0931	0.3542	0.1828	0.83	single atom P
O3	6 <i>l</i>	1	0.1249	0.101	0.3418	0.18	non-colinear O ₂
O4	6 <i>l</i>	1	0.3394	0.2623	0.3283		non-colinear PO
Ca5	3 <i>k</i>	<i>m</i> ..	0.0111	0.2608	¹ / ₂	0.95	non-colinear O ₂
O6	3 <i>k</i>	<i>m</i> ..	0.3288	0.4843	¹ / ₂	0.84	single atom P
P7	3 <i>k</i>	<i>m</i> ..	0.4015	0.3715	¹ / ₂	0.89	tetrahedron O ₄
O8	3 <i>k</i>	<i>m</i> ..	0.5305	0.1151	¹ / ₂		single atom P
P9	3 <i>j</i>	<i>m</i> ..	0.0311	0.4019	0	0.95	tetrahedron O ₄
O10	3 <i>j</i>	<i>m</i> ..	0.1252	0.5875	0	0.97	single atom P
Ca11	3 <i>j</i>	<i>m</i> ..	0.259	0.2483	0	0.96	
O12	3 <i>j</i>	<i>m</i> ..	0.4853	0.1527	0		single atom P
Ca13	2 <i>i</i>	3..	² / ₃	¹ / ₃	0.2487		octahedron O ₆
Ca14	2 <i>h</i>	3..	¹ / ₃	² / ₃	0.2538	0.89	tricapped trigonal prism O ₉
O15	2 <i>g</i>	3..	0	0	0.0642	0.55	
C16	2 <i>g</i>	3..	0	0	0.2491	0.54	7-vertex polyhedron O ₇

Transformation from published data: -*y*, -*x*, -*z*

Experimental: single crystal, diffractometer, X-rays, $wR = 0.027$

Remarks: The occupancies of sites Ca13, O4, O8, and O12 were set to unity (published values 1.02, 1.11, 1.05, and 1.17, respectively). Short interatomic distances for partly occupied site(s).

References: [1] Suetsugu Y., Takahashi Y., Okamura P., Tanaka J. (2000), J. Solid State Chem. 155, 292-297.