$Ca_{9.75}[PO_4]_{5.5}[CO_3]_{1.5}$	*hP*56	(174) *P*-6 – $l^4k^4j^4ihg^2$

$Ca_{9.75}(PO_4)_{5.5}(CO_3)_{1.5}$ [1], apatite family
Structural features: Infinite columns of base-linked CaO_6O_3 tricapped trigonal prisms share atoms with PO_4 tetrahedra to form a 3D-framework (partial vacancies ignored); CO_3 trigonal units in infinite columns of face-linked Ca_6 octahedra parallel to [001] (units parallel to [001], partial orientational disorder).

Suetsugu Y. et al. (2000) [1]
$C_{1.08}Ca_{9.51}O_{25.67}P_{5.52}$
a = 0.948, c = 0.6898 nm, c/a = 0.728, V = 0.5369 nm^3, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6*l*	1	0.0276	0.1271	0.3411	0.18	non-colinear O_2
O2	6*l*	1	0.0931	0.3542	0.1828	0.83	single atom P
O3	6*l*	1	0.1249	0.101	0.3418	0.18	non-colinear O_2
O4	6*l*	1	0.3394	0.2623	0.3283		non-colinear PO
Ca5	3*k*	*m*..	0.0111	0.2608	$^1/_2$	0.95	non-colinear O_2
O6	3*k*	*m*..	0.3288	0.4843	$^1/_2$	0.84	single atom P
P7	3*k*	*m*..	0.4015	0.3715	$^1/_2$	0.89	tetrahedron O_4
O8	3*k*	*m*..	0.5305	0.1151	$^1/_2$		single atom P
P9	3*j*	*m*..	0.0311	0.4019	0	0.95	tetrahedron O_4
O10	3*j*	*m*..	0.1252	0.5875	0	0.97	single atom P
Ca11	3*j*	*m*..	0.259	0.2483	0	0.96	
O12	3*j*	*m*..	0.4853	0.1527	0		single atom P
Ca13	2*i*	3..	$^2/_3$	$^1/_3$	0.2487		octahedron O_6
Ca14	2*h*	3..	$^1/_3$	$^2/_3$	0.2538	0.89	tricapped trigonal prism O_9
O15	2*g*	3..	0	0	0.0642	0.55	
C16	2*g*	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.