

$\text{Na}_{0.4}\text{Ca}_{4.2}[\text{PO}_4]_{1.8}[\text{CO}_3]_{1.2}[\text{OH}]$	<i>hP80</i>	(176) $P6_3/m - i^3h^6fe$
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$\text{Na}_{0.8}\text{Ca}_{8.4}(\text{PO}_4)_{3.6}(\text{CO}_3)_{2.4}(\text{OH})_2$ [1], apatite family

Structural features: Infinite columns of base-linked CaO_6O_3 tricapped trigonal prisms (partial substitution and vacancies ignored) share atoms with PO_4 tetrahedra and CO_3 trigonal units (substitutional disorder, orientational disorder for the latter) to form a 3D-framework; OH in infinite columns of face-linked $(\text{Ca},\text{Na})_6$ octahedra parallel to [001] (partial disorder).

El Feki H. et al. (2000) [1]

$\text{C}_{1.20}\text{Ca}_{4.20}\text{HNa}_{0.39}\text{O}_{11.80}\text{P}_{1.80}$

$a = 0.93249$, $c = 0.69213$ nm, $c/a = 0.742$, $V = 0.5212$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.327	0.074	0.0678	0.6	
O2	12 <i>i</i>	1	0.41	0.126	0.045	0.2	
C3	12 <i>i</i>	1	0.429	0.031	0.174	0.2	
O4	6 <i>h</i>	<i>m..</i>	0.121	0.47	$\frac{1}{4}$	0.4	
O5	6 <i>h</i>	<i>m..</i>	0.167	0.486	$\frac{1}{4}$	0.6	
M6	6 <i>h</i>	<i>m..</i>	0.2439	0.26	$\frac{1}{4}$	0.959	
P7	6 <i>h</i>	<i>m..</i>	0.3934	0.0249	$\frac{1}{4}$	0.6	
O8	6 <i>h</i>	<i>m..</i>	0.569	0.101	$\frac{1}{4}$	0.4	
O9	6 <i>h</i>	<i>m..</i>	0.586	0.134	$\frac{1}{4}$	0.6	
M10	4 <i>f</i>	3.. <i></i>	$\frac{1}{3}$	$\frac{2}{3}$	0.0003	0.861	tricapped trigonal prism O ₉
(OH)11	4 <i>e</i>	3.. <i></i>	0	0	0.14	0.5	single atom (OH)

M6 = 0.875Ca + 0.125Na; M10 = 0.98Ca + 0.02Na

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

Experimental: powder, diffractometer, X-rays, R = 0.041

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 8 of [1] the *y*-coordinate of former Oc(3) is misprinted as 0284 instead of 0.284.

References: [1] El Feki H., Savariault J.M., Ben Salah A., Jemal M. (2000), Solid State Sci. 2, 577-586.