

$\text{Na}_{7.2}(\text{Al}_{0.4}\text{Si}_{0.6})_{12}[\text{CO}_3]_{1.2}\text{O}_{24}[\text{H}_2\text{O}]_3$ 
*hP84*

(186)  $P6_3mc - d^2c^8b^3a^3$ 
 **$\text{Na}_{7.2}\text{Al}_{4.8}\text{Si}_{7.2}\text{O}_{24}(\text{CO}_3)_{1.2} \cdot 3\text{H}_2\text{O}$**  [1], zeolite CAN- $\text{CO}_3$ 

Structural features: (Si,Al) $\text{O}_4$  tetrahedra share vertices to form a CAN-type zeolite framework with channels delimited by 12-rings perpendicular to [001];  $\text{H}_2\text{O}$  at the centers of cancrinite-type cages (11-face polyhedra formed by six 4-rings, two planar and three non-planar 6-rings),  $\text{CO}_3$  trigonal units (orientational disorder) in the channels, Na above 6-rings in cages and channels.

Khomyakov A.P. et al. (1991) [1]

 $\text{Al}_{4.80}\text{C}_{1.22}\text{H}_6\text{Na}_{7.28}\text{O}_{31.08}\text{Si}_{7.20}$ 
 $a = 1.2575$ ,  $c = 0.5105$  nm,  $c/a = 0.406$ ,  $V = 0.6991$  nm<sup>3</sup>,  $Z = 1$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	12 <i>d</i>	1	0.0793	0.4122	0.2112		tetrahedron O <sub>4</sub>
O2	12 <i>d</i>	1	0.3566	0.0356	0.0122		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )3	6 <i>c</i>	. <i>m</i> .	0.058	0.942	0.422	0.17	
O4	6 <i>c</i>	. <i>m</i> .	0.0598	0.9402	0.34	0.31	
O5	6 <i>c</i>	. <i>m</i> .	0.06	0.94	0.148	0.37	
O6	6 <i>c</i>	. <i>m</i> .	0.2022	0.7978	0.1246		non-colinear Si <sub>2</sub>
O7	6 <i>c</i>	. <i>m</i> .	0.4421	0.5579	0.1849		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )8	6 <i>c</i>	. <i>m</i> .	0.648	0.352	0.16	0.18	
Na9	6 <i>c</i>	. <i>m</i> .	0.86	0.14	0.252	0.1	
Na10	6 <i>c</i>	. <i>m</i> .	0.8775	0.1225	0.2452	0.85	
Na11	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.043	0.24	
Na12	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.119	0.55	
(OH <sub>2</sub> )13	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.62	0.29	
(OH <sub>2</sub> )14	2 <i>a</i>	3 <i>m</i> .	0	0	0.0	0.16	
C15	2 <i>a</i>	3 <i>m</i> .	0	0	0.152	0.31	
C16	2 <i>a</i>	3 <i>m</i> .	0	0	0.351	0.3	

M1 = 0.6Si + 0.4Al

Transformation from published data: origin shift 0 0 0.54

Experimental: single crystal, diffractometer, X-rays, R = 0.029

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Khomyakov A.P., Pobedinskaya E.A., Nadezhina T.N., Terent'eva L.E., Rastsvetaeva R.K. (1991), Vestn. Mosk. Univ., Ser. 4: Geol. 1991(5), 79-84.