

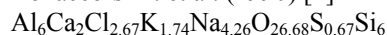
hP94

(176) $P6_3/m - i^4h^7ca$

K₂Na₄Ca₂Al₆Si₆O₂₄(SO₄)Cl₂ [1], davyne, zeolite CAN-Cl,SO₄

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a CAN-type zeolite framework with channels delimited by 12-rings perpendicular to [001]; Cl near the centers of cancrinite-type cages (11-face polyhedron formed by six 4-rings, two planar and three non-planar 6-rings), Ca at the centers of planar 6-rings, additional Cl, SO₄ tetrahedra (orientational disorder), Na and K in the channels.

Bonaccorsi E. et al. (1990) [1]



$a = 1.2705$, $c = 0.5368$ nm, $c/a = 0.423$, $V = 0.7504$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.0087	0.3317	0.0084		non-colinear SiAl
O2	12 <i>i</i>	1	0.02	0.04	0.02	0.056	
Cl3	12 <i>i</i>	1	0.049	0.009	0.075	0.056	
O4	12 <i>i</i>	1	0.1132	0.0701	0.1254	0.167	
Si5	6 <i>h</i>	<i>m</i> ..	0.0809	0.4093	¹ / ₄		tetrahedron O ₄
O6	6 <i>h</i>	<i>m</i> ..	0.1002	0.5435	¹ / ₄		non-colinear SiAl
O7	6 <i>h</i>	<i>m</i> ..	0.2162	0.4307	¹ / ₄		non-colinear SiAl
M8	6 <i>h</i>	<i>m</i> ..	0.2217	0.1081	¹ / ₄	0.5	
Na9	6 <i>h</i>	<i>m</i> ..	0.3097	0.151	¹ / ₄	0.5	
Al10	6 <i>h</i>	<i>m</i> ..	0.3395	0.4086	¹ / ₄		tetrahedron O ₄
Cl11	6 <i>h</i>	<i>m</i> ..	0.6372	0.315	¹ / ₄	0.333	
Ca12	2 <i>c</i>	-6..	¹ / ₃	² / ₃	¹ / ₄		
S13	2 <i>a</i>	-6..	0	0	¹ / ₄	0.333	

M8 = 0.58K + 0.42Na

Transformation from published data: *y,x,-z*; origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.049

Remarks: Natural specimen from Monte Somma, Vesuvius area, Italy. Composition (Na_{4.36}K_{1.49}Ca_{2.15})₂(Si_{5.93}Al_{6.07}O_x)(SO₄)_{0.61}Cl_{2.93} from electron microprobe analysis. Short interatomic distances for partly occupied site(s). In table 2 of [1] the *z*-coordinate of former site Na is misprinted as ³/₄ instead of ¹/₄ (checked on interatomic distances).

References: [1] Bonaccorsi E., Merlino S., Pasero M. (1990), Neues Jahrb. Mineral., Monatsh. 1990, 97-112.