

(Na,K)₆Ca₂Al₆Si₆O₂₄Cl₄ [1], quadridavyne, zeolite CAN-Cl

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 at 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, Na and K in the channels (partly ordered arrangement causing the supercell).

Bonaccorsi E. et al. (1994) [1]

Al₂₄Ca₈Cl₁₆K_{7.66}Na_{16.34}O₉₆Si₂₄

$a = 2.5771$, $c = 0.5371$ nm, $c/a = 0.208$, $V = 3.0892$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.005	0.333	0.021		non-colinear AlSi
O2	12i	1	0.163	0.494	0.008		non-colinear SiAl
O3	12i	1	0.172	0.17	0.02		non-colinear SiAl
O4	12i	1	0.511	0.174	0.007		non-colinear SiAl
Cl5	6h	m..	0.018	0.047	1/4	0.167	
Cl6	6h	m..	0.018	0.547	1/4		single atom K
Cl7	6h	m..	0.042	0.024	1/4	0.167	
Na8	6h	m..	0.048	0.439	1/4		non-coplanar square O ₄
M9	6h	m..	0.054	0.106	1/4	0.38	
M10	6h	m..	0.071	0.139	1/4	0.36	
M11	6h	m..	0.091	0.182	1/4	0.26	
Cl12	6h	m..	0.1561	0.313	1/4		non-coplanar triangle Ca ₂ Na
Si13	6h	m..	0.2049	0.1615	1/4		tetrahedron O ₄
Al14	6h	m..	0.2082	0.0345	1/4		tetrahedron O ₄
Al15	6h	m..	0.209	0.5398	1/4		tetrahedron O ₄
O16	6h	m..	0.215	0.105	1/4		non-colinear SiAl
O17	6h	m..	0.22	0.612	1/4		non-colinear SiAl
O18	6h	m..	0.273	0.211	1/4		single atom Si
O19	6h	m..	0.277	0.553	1/4		non-colinear AlSi
O20	6h	m..	0.2844	0.06	1/4		non-colinear SiAl
K21	6h	m..	0.317	0.409	1/4		trigonal prism O ₆
Si22	6h	m..	0.3326	0.5408	1/4		tetrahedron O ₄
Al23	6h	m..	0.333	0.299	1/4		tetrahedron O ₄
Ca24	6h	m..	0.334	0.165	1/4		hexagonal bipyramid O ₆ Cl ₂
Si25	6h	m..	0.335	0.041	1/4		tetrahedron O ₄
O26	6h	m..	0.398	0.106	1/4		non-colinear SiAl
O27	6h	m..	0.399	0.294	1/4		non-colinear SiAl
O28	6h	m..	0.445	0.223	1/4		non-colinear SiAl
Si29	6h	m..	0.4597	0.2921	1/4		tetrahedron O ₄
Al30	6h	m..	0.464	0.168	1/4		tetrahedron O ₄
Na31	6h	m..	0.587	0.173	1/4		non-colinear O ₂
Cl32	2d	-6..	2/3	1/3	1/4		colinear Ca ₂
Ca33	2c	-6..	1/3	2/3	1/4		hexagonal bipyramid O ₆ Cl ₂

M9 = 0.74Na + 0.26K; M10 = 0.67Na + 0.33K; M11 = 0.77Na + 0.23K

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

Experimental: single crystal, diffractometer, X-rays, R = 0.140

Remarks: Natural specimen from Ottaviano, Vesuvius area, Italy. Composition Na_{3.97}K_{1.38}Ca_{2.22}Al_{5.95}Si_{6.05}O_{23.90}(SO₄)_{0.15}Cl_{3.76} from electron microprobe analysis. Diffraction data from several crystals were combined. Short interatomic distances for partly occupied site(s). In table 3 of [1] the y-coordinate of

former Cl1 is misprinted as $\frac{1}{4}$ instead of $\frac{1}{3}$; the site multiplicity and occupancy of former Ca2 and Cl2 are misprinted as 1 and $\frac{1}{6}$ instead of $\frac{1}{6}$ and 1 (fully occupied Wyckoff position $6h$), respectively.

References: [1] Bonaccorsi E., Merlino S., Orlandi P., Pasero M., Vezzalini G. (1994), Eur. J. Mineral. 6, 481-487.