COMPILATION OF EXTRA FRAMEWORK SITES IN ZEOLITES

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PREFACE

The scientific understanding of the physico-chemical properties of zeolites is strongly related to the underlying crystal structure. The key structural information consists not only in the structure type, but also in the distribution of the cations and extra-framework species in the zeolite cavities and channels. Because of the steadily growing number of published structures, many of them varying only in the content of exchangeable cations and guest molecules, the Structure Commission of the International Zeolite Association has felt the need for a condensed compilation.

A total of 36 structure types were selected for this atlas and all literature references available to me by the Spring of 1981 (or kindly supplied by the authors prior to publication) are included. It is the aim of the IZA Structure Commission to update this compilation from time to time in the future. If I have overlooked some references, or made some errors, I apologize for it and I hope that the authors are so kind to inform me of this shortcoming. The reader is urged not to rely uniquely on this atlas, but to consult also the original papers since a compilation of this type inevitably requires several generalizations.

I wish to thank my colleagues of the IZA Structure Commission for critically reading the manuscript and for many helpful comments. I hereby wish to acknowledge especially the suggestion made by the late Dr. D.W. Breck to include all literature data in this atlas.

I'm indebted to the "Belgisch Nationaal Fonds voor Wetenschappelijk Onderzoek" (N.F.W.O.) for a research position as "Bevoegdverklaard Navorser" (Research Associate) and to the Catholic University of Leuven (K.U.Leuven) for research facilities and financing. Finally, but not perfunctorily, I wish to thank Hilda Meeus for her patience and diligence in preparing the camera-ready copy.

Wilfried J. MORTIER

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EXPLANATORY NOTES

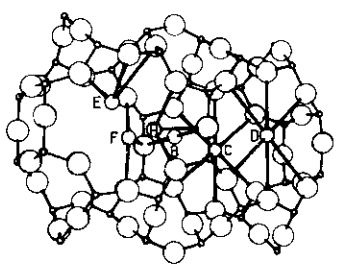
SAMPLE PAGE

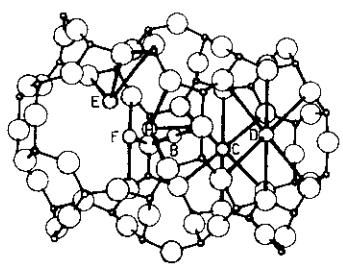
The bold figures refer to the same figures placed between squared brackets in the text.

EPI

(2)

(3)





(1) EPISTILBITE

EPISTILBITE

Framework EPI = $[Al_xSi_{24-x}O_{48}]$ (4) x = 6.5 (5) C2/m (6) V = 1350 Å^3 (7)

Extra-framework sites :

(8) site	(9) type	(10) site symmetry	(11) coordination distances (Å)
A	IV8	m[C_s]	2x2.58 2.60
B	IV8	2/m[C_{2h}]	2x3.03
C	III8	2/m[C_{2h}]	4x3.13 2x3.19
D	III8	2/m[C_{2h}]	2x3.18 4x3.43
E	IV8	1	3.09 3.18 3.46
F	IV8	m[C_s]	2.43 2x2.90

Site occupancies :

(8) site :	A	B	C	D	E	F
(12) (1)	xCa,Na	(13) xH_2O***	xH_2O	-	xH_2O	xH_2O
(2)	2.3Ca	$0.6H_2O$, $2.8H_2O$***	$2H_2O$	$2H_2O$	$4H_2O$, $4H_2O$	$0.6Ca$, $0.5H_2O$

(12) (14) (15) (16)

*(1) $Ca_{2.6}Na_{1.1}K_{0.1}$[6.3].15.7H_2O; h; a = 9.08 b = 17.74 c = 10.25 β = 124.9°
A.J. Perrotta, Min. Mag., 36, 480 (1967).

(2) $Ca_{2.7}Na_{0.4}Mg_{0.1}$[6.5].15H_2O; h; C2 a = 9.04 b = 17.75 c = 9.08 β = 111.8°
[0, 1, 0, -1; 0, 0, 1, 0; 1/2, 0, 0, -1] (17)
M. Slaughter, W.T. Kane, Zeit. Kristallogr., 130, 68 (1969). (18)

1. Name of type species.
2. Mnemonic code.
3. Stereo plots.
4. Framework composition (no./unit cell).
5. Typical number of Al/unit cell.
6. Typical space group.
7. Unit cell volume.
8. Site indication, referring to the same sequential lettering in the stereo plots.
9. Site type including information on coordination and accessibility.
10. Site symmetry in the typical space group (6).

11. Coordination distances of the sites shown in the stereo plots (indicative, unless underlined which means fixed by symmetry).
12. Reference sequence number.
13. Occupancies : no./unit cell and species located, eventually marked with one or two asterisks.
14. Compositional formula.
15. Pretreatment conditions.
16. Space group (not given if identical with 6) and unit cell parameters.
17. Transformation matrix to transform the coordinates to those of the structure for which the reference number is marked with an asterisk.
18. Reference and pertinent comments if necessary.

STRUCTURE TYPES

The type structures [1], chosen for this compilation were those described in the "Atlas of Zeolite Structure Types" by W.M. Meier and D.H. Olson (1978). Isotypic zeolite species which do not differ with respect to their framework topology are classified with the same type species, irrespective of their composition, ordering of the tetrahedral framework atoms, cell dimensions and symmetry. The same mnemonic code [2] consisting of three capital letters has been adopted as used before by Meier and Olson, hereby following the IUPAC recommendations (R.M. Barrer, Pure & Appl. Chem., 51, 1091 (1979)). The various structure types have been arranged in alphabetic order according to the structure type code.

THE STEREO PLOTS

For each structure type, the drawings [3] display all possible types of cages, channels and framework rings. The ball-and-stick model was chosen, with the tetrahedral framework atoms represented by the smallest spheres and the framework oxygens by the largest. The extra-framework sites are shown by intermediate-sized spheres and their coordination to the framework is demonstrated by heavy stick bonds to the nearest oxygens (maximum distance : 3.5 Å). The positions of the sites (cations and guest molecules) are those described in the literature as they were obtained by X-ray and neutron-diffraction methods. Hypothetical sites such as the centers of the framework rings are also considered. The stereo plots were prepared with the use of the stereographic plotting program ORTEP, written by C.K. Johnson (Oak Ridge National Laboratory, U.S.A.).

SUMMARY OF STRUCTURAL DATA

The typical framework composition [4] is placed in square brackets and given in numbers per unit cell, with the typical number of tetrahedral Al atoms [5] given separately. The space group [6] of the type structure which was used to establish the framework drawing is also included, together with its unit cell volume [7]. This type structure was preferably chosen as the hydrated mineral for which single crystal data were available.

Furthermore, a table with a more detailed description of the sites using the same sequential lettering [8] as in the stereo-drawings is given. The site type [9] informs on the coordination type and the accessibility. The site symmetry [10] is for the space group of the type species under consideration. The coordination distances [11] are those for the bonds shown. If fixed by symmetry, the distances are underlined. The other distances are only indicative and depend on the actual location.

The following conventions were adopted for characterizing the site types [9]. The extra-framework sites are analysed according to two different criteria which are included in the site type code.
(i) The type of coordination with the framework is indicated by a Roman numeral (I-V).

(ii) The accessibility of the site in terms of the type of framework ring limiting the cage or channel entrance is designated by the number of TO_4 tetrahedra in the limiting ring.

The following coordination types are considered :

I hexagonal prism site

II single six-ring site

III eight-ring site

IV all other sites with framework oxygens in the first coordination sphere

V sites without framework oxygens in the first coordination sphere.

NOTE : if a site meets the criteria for two coordination types, the first classified type dominates.

NOTE : the hexagonal prism is unequivocally defined by its site type and does not need any further specification on accessibility.

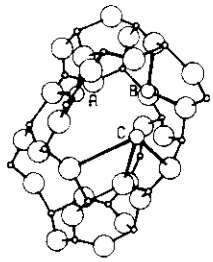
LITERATURE SURVEY

A first table comprises the occupancies [13] (no./unit cell) and type of species located (indicated by the chemical symbol or M for undefined cations, Ø for "oxygen species", and X for undefined oxygen, water or cationic species). Cases marked with one asterisk (*) indicate atoms slightly displaced (up to 1 Å) from the symmetry element of the site. A site shifted by more that 1 Å from the site displayed in the stereo plot is marked by two asterisks.

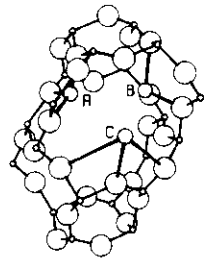
The reference list [12] includes the unit cell composition [14]; the pretreatment conditions [15]; the space group [16] (not given if identical with the one of the type structure) and the unit cell parameters [16]; the transformation matrix [17] for the coordinates if necessary and if required, some pertinent comments [18]. The compositional formula [14] contains the cations, the number of tetrahedral Al atoms per unit cell in squared brackets (this refers to x in the structural formula of the framework), and followed by the amount and type of guest species. The pretreatment conditions [15] are indicated by h for hydrated, d for dehydrated, a + sign for successive treatments, and eventually the type of guest molecules adsorbed. The transformation matrix [17] to transform the coordinates to those of the type structure (marked with an asterisk before the reference sequence number if this applies) is defined as : $[t_1, s_{11}, s_{12}, s_{13}; t_2, s_{21}, s_{22}, s_{23}; t_3, s_{31}, s_{32}, s_{33}]$, such that the transformed coordinates x', y', z' are obtained by

$$x' = t_1 + s_{11}.x + s_{12}.y + s_{13}.z$$
$$y' = t_2 + s_{21}.x + s_{22}.y + s_{23}.z$$
$$z' = t_3 + s_{31}.x + s_{32}.y + s_{33}.z$$

ABW



LI-A (BW)



LI-A (BW)

Framework ABW = $[Al_xSi_{8-x}O_{16}]$ x = 4 $Pna2_1$ V = 422 $\AA^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)		
A	II8	1	1.8	2.1	2.2
B	II8	1	1.9	2.4	2.0
C	III8	1	3.0	3.1	3.4

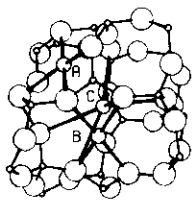
Site occupancies :

site :	A	B	C
(1)	2.2Li	1.7Li	$3.9H_2O$
(2)	2.6Li	1.1Li	$3.9H_2O$

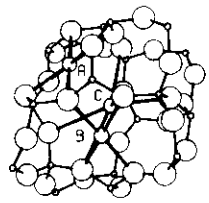
(1) $Li_{3.5}[3.9].8H_2O$; h; a = 10.3 b = 8.2 c = 5.0
I.S. Kerr, "Molecular Sieves", J.B. Uytterhoeven, ed., Proc. 3rd Int. Conf. on Molecular Sieves, Leuven University Press (Belgium) (1973), p. 104.

(2) $Li_{3.5}[3.9].8H_2O$; h; a = 10.3 b = 8.2 c = 5.0
I.S. Kerr, Z. Kristallogr., 139, 186 (1974).

ANA



ANALCIME



ANALCIME

Framework ANA = $[Al_xSi_{48-x}O_{96}]$ x = 16 Ia3d V = 2571 $\mathring{A}^3$

Extra-framework sites :

site	type	site symmetry	coordination distances ($\mathring{A}$)
A	II8	$\bar{3}[S_6]$	6x2.59
B	III8	$222[D_2]$	4x2.50
C	IV8	$32[D_3]$	6x3.41

Site occupancies :

site :	A	B	C
(1)	-	16Na	$16H_2O$
(2)	-	-	16Cs
(3)	-	16Na	$16H_2O$
(4)a.	-	16Na	$16H_2O$
b.	-	16Na	$16H_2O$
(5)	-	$4H_2O$	16(Cs,Na)
(6)	-	-	$16(Cs,Na,H_2O)$
(7)	-	-	16K
(8)	-	4(Na or H_2O)	12Cs, 4(H_2O or Na)
(9)	-	16Na	$16H_2O$
(10)a.	-	13.1Na*, 1.8Na	$16H_2O$*
b.	-	13.4Na*, 1.4Na	$16H_2O$*
c.	-	12.6Na*, 3.8Na	$16H_2O$*
d.	-	5.9Na*, 5.9Na*, 4.2Na*	$16H_2O$*
e.	-	11.7Na*, 4.6Na	$16H_2O$*
f.	-	9.9Na*, 6.2Na	$16H_2O$*
g.	-	5.5Na*, 4.2Na*, 6.4Na*	$16H_2O$*

(1) $Na_{16}[16].16H_2O$; h; a = 13.7
W.H. Taylor, Z. Kristallogr., 74, 1 (1930).

(2) $Cs_{16}[16].xH_2O$; h; I4/acd a = 13.74 c = 13.74
S. Von Naray Szabo, Z. Kristallogr., 99, 277 (1938).

(3) $Na_{16}[16].16H_2O$; h; a = 13.73
M. Calleri, G. Ferraris, Atti della Academia della Science di Torino, 98, 424 (1964).

(4) a. $K_{0.4}Na_{15.5}[16].16H_2O$; h; a = 13.73
b. $K_{0.3}Na_{15.0}[16].16H_2O$; h; a = 13.73
C.R. Knowles, F.F. Rinaldi, J.V. Smith, The Indian Mineralogist, 6, 127 (1965).

(5) $Cs_{12}Na_4[16].4H_2O$; h; a = 13.69
R.M. Beger, M.J. Buerges, Proc. Nat. Acad. Sci. U.S., 58, 853 (1967).

(6) $Cs_{11.2}Na_{4.8}[16].4.8H_2O$; h; a = 13.68
R.E. Newnham, Amer. Mineral., 52, 1515 (1967).

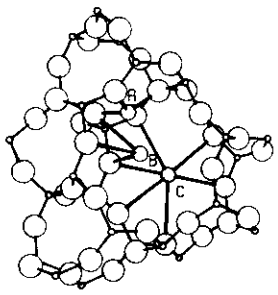
(7) $K_{13.6}Na_{2.4}[16]$; d, at 908K; a = 13.7
D.R. Peacor, Z. Kristallogr., 127, 213 (1968).

(8) $Cs_{12}Na_4[16].4H_2O$; h; a = 13.69
R.M. Beger, Z. Kristallogr., 129, 280 (1969).

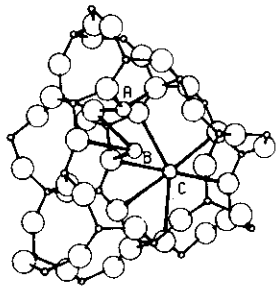
(9) $Na_{16}[16].16H_2O$; h; a = 13.73
[protons located]
G. Ferraris, D.W. Jones, J. Yerkess, Z. Kristallogr., 135, 240 (1972).

(10) a. $Na_{14.8}K_{0.0}Ca_{0.0}[15.4].16H_2O$; h; $I4_1/acd$ a = 13.72 c = 13.69
b. $Na_{14.9}K_{0.0}Ca_{0.0}[15.3].16H_2O$; h; $I4_1/acd$ a = 13.73 c = 13.69
c. $Na_{15.7}K_{0.1}Ca_{0.0}[16.1].16H_2O$; h; $I4_1/acd$ a = 13.73 c = 13.71
d. $Na_{15.7}K_{0.1}Ca_{0.0}[15.7].16H_2O$; h; Ibca a = 13.73 b = 13.73 c = 13.71
e. $Na_{15.4}K_{0.1}Ca_{0.1}[16.1].16H_2O$; h; $I4_1/acd$ a = 13.73 c = 13.72
f. $Na_{15.2}K_{0.1}Ca_{0.6}[16.3].16H_2O$; h; $I4_1/acd$ a = 13.72 c = 13.74
g. $Na_{15.7}K_{0.1}Ca_{0.0}[15.6].16H_2O$; h; Ibca a = 13.73 b = 13.71 c = 13.74
F. Mazzi, E. Galli, Amer. Mineral., 63, 448 (1978).

BIK



BIKITAITE



BIKITAITE

Framework BIK = $[Al_xSi_{6-x}O_{12}]$ x = 2 $P2_1$ V = 298 $Å^3$

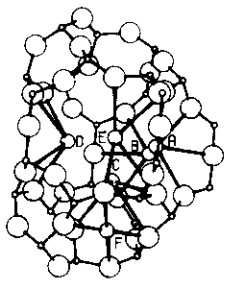
Extra-framework sites :

site	type	site symmetry	coordination distances (Å)		
A	II8	1	1.9	2.0	2.0
B	IV8	1	3.1	3.2	3.2
C	III8	1	2x3.0	3.1	3.3
			3.4	3.5	

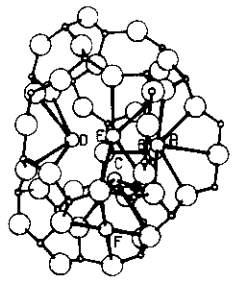
Site occupancies :

site :	A	B	C
(1)	2Li	$2H_2O$	-

(1) $Li_2[2].2H_2O$; h; a = 8.6 b = 5.0 c = 7.6 β = 114°
V. Kocman, R.I. Gait, J. Rucklidge, Am. Mineral., 59, 71 (1974).



BREWSTERITE



BREWSTERITE

Framework BRE = $[Al_xSi_{16-x}O_{32}]$ x = 4 $P2_1/m$ V = 915 $Å^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	III8	m[C_s]	2x2.85 2x2.87 3.20
B	III8	m[C_s]	2x2.98 3.30
C	IV8	1	3.27 3.29 3.33 3.40
D	III8	m[C_s]	2x3.05 2x3.17
E	IV8	m[C_s]	2x2.89 2x3.35
F	II8	$\bar{1}$[C_i]	2x2.29 2x2.53

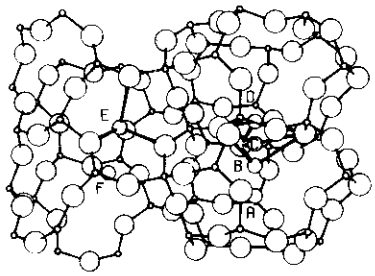
Site occupancies :

site :	A	B	C	D	E	F
(1)	2Sr	$2H_2O$	$4H_2O$	$2H_2O$	$2H_2O$	-
(2)	2Sr,Ba	$2H_2O$	$4H_2O$	$2H_2O$	$2H_2O$	-

(1) $(Sr,Ca,Ba)_2[4].10H_2O$; h; a = 6.77 b = 17.51 c = 7.74 β = 94.3°
A.J. Perrotta, J.V. Smith, Acta Crystallogr., 17, 857 (1964).

(2) $Ba_{0.5}Sr_{1.5}[4].10H_2O$; h; a = 6.79 b = 17.57 c = 7.76 β = 94.54°
J.L. Schlenker, J.J. Pluth, J.V. Smith, Acta Crystallogr., B33, 2907 (1977).

CAN



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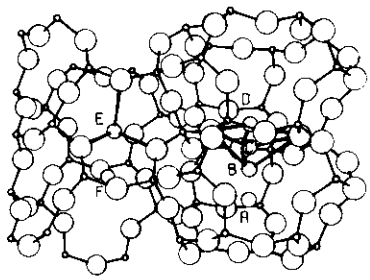


CANCRINITE

Framework CAN = $[Al_xSi_{12-x}O_{24}]$ x = 6 $P6_3$ V = 724 $\AA^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	V6	$3[C_3]$	-
B	II6	$3[C_3]$	3x2.8
C	II6	$3[C_3]$	3x2.5
D	II6	$3[C_3]$	3x2.5
E	II12	1	2.4 2.5 2.7
F	VI2	$3[C_3]$	-

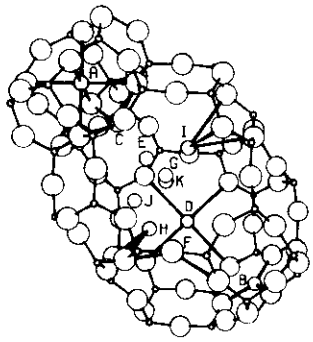
Site occupancies :

site :	A	B	C	D	E	F
(1)	$2H_2O$:::	2(Na,Ca)	-	-	$6(Na_2,Ca)$	1C::: 3Ø:::
(2)a.	1.8Ø	-	1.4Na	-	4.2Na 1.5Na	1Ø 2.6Ø::: 2.2Ø:::
b.	2.5Ø:::	1.6Ø	0.9Ø	1.1Na	5.2Na	1.8Na

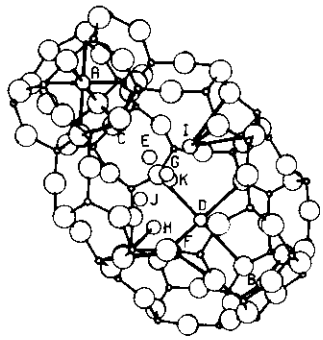
(1) $Na_{6.3}[6].Ca_{0.9}Fe_{0.1}(CO_3)_{1.5}.2.5H_2O$; h; a = 12.75 c = 5.14
O. Jarchow, Z. Kristallogr., 122, 407 (1965).

(2) a. $Na_6[6].1.1SiO_2.0.6Na_2O.4.1H_2O$; h; a = 12.72 c = 5.19
b. $Na_6[6].1.9NaNO_3.1.44H_2O$; h; a = 12.67 c = 5.19
R.M. Barrer, J.F. Cole, H. Villiger, J. Chem. Soc., 1523 (1970).

CHA



CHABAZITE



CHABAZITE

Framework CHA = $[Al_xSi_{12-x}O_{24}]$ x = 4 $R\bar{3}m$ V = 825 $\AA^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	I	$\bar{3}m[D_{3d}]$	6x2.60
B	II8	$3m[C_{3v}]$	3x2.13
C	II8	$3m[C_{3v}]$	3x2.40
D	III8	$2/m[C_{2h}]$	2x3.10 2x3.34
E	V8	$3m[C_{3v}]$	-
F	IV8	1	2.55 2.58 3.05
G	V8	$m[C_s]$	-
H	IV8	$2[C_2]$	2.91 2x3.31
I	IV8	$m[C_s]$	3.24 2x3.27
J	V8	$m[C_s]$	-
K	V8	$3m[C_{3v}]$	-

Site occupancies :

site :	A	B	C	D	E	F	G	H	I	J	K
(1)	0.6Ca	-	0.4Ca	-	-	-	-	-	-	-	-
(2)	-	-	$2H_2O$	$3H_2O$	-	-	-	2Ca*	$6H_2O$	-	$2H_2O$
(3)a.	-	-	$2H_2O$	$3H_2O$	-	-	-	2Ca*	$6H_2O$	-	$2H_2O$
b.	-	-	$2H_2O$	$3H_2O$	-	-	-	2Ca*	$6H_2O$	-	$2H_2O$
(4)a.	0.3Ca	-	1.2Ca	-	-	-	-	-	-	4Cl	-
b.	-	-	2.0Ca	-	-	-	-	-	-	6Cl*	-
c.	-	-	2.0Ca	-	-	-	-	-	-	6Cl*	-
(5)	0.1Ca	-	1.9Ca	-	-	-	-	-	-	-	-
(6)	0.1Ca	-	1.8Ca	-	1.8C*	-	-	-	-	1.8Ø*	-
(7)	0.4Na*	-	2.7Na* 3.2Na*	3.8Na* 3.2Na* 1.9Na* 0.4Na*	-	-	-	-	-	-	-
(8)a.	-	1.8Cu	-	-	-	-	-	-	-	-	-
b.	-	-	$2.3H_2O$	$3H_2O$	-	0.7Cu	0.5Cu	$4.2H_2O$	$7.4H_2O$	-	-
(9)a.	0.3Ca	-	-	-	-	-	-	-	-	-	-
b.	0.2Ca	-	-	-	-	-	-	-	-	-	-
(10)	0.1(Ca,Sr)	-	1.1(Ca,Sr)	$1.5H_2O$	-	-	$3.4H_2O$	-	$2.8H_2O$*	-	0.5(Ca,Sr)

CHA

(1) $Ca_{1.95}$[3.9]; d; a = 9.37 α = 92°
[+ 0.75 Ca at uncertain general position]
J.V. Smith, Acta Crystallogr., 15, 835 (1962).

(2) $Ca_{1.95}$[3.9].13H_2O; h; a = 9.42 α = 94.5°
J.V. Smith, F. Rinaldi, L.S. Dent Glasser, Acta Crystallogr., 16, 45 (1963).

(3) a. $Ca_{1.95}$[3.9].13H_2O; h; a = 9.45 α = 94.5°
b. $Ca_{1.95}$[3.9].13H_2O; h (123K); a = 9.45 α = 94.7°
J.V. Smith, C.R. Knowles, F. Rinaldi, Acta Crystallogr., 17, 374 (1964).

(4) a. $Ca_{1.95}$[3.9].xCl_2; d + Cl_2; a = 9.45 α = 95.4°
b. $Ca_{1.95}$[3.9].xCl_2; d + Cl_2; a = 9.45 α = 95.2°
c. $Ca_{1.95}$[3.9].xCl_2; d + Cl_2 (123K); a = 9.45 α = 95.2°
J.H. Fang, J.V. Smith, J. Chem. Soc., 3749 (1964).

(5) $Ca_{1.9}$[3.8]; d; a = 9.44 α = 93.1°
W.J. Mortier, J.J. Pluth, J.V. Smith, Mat. Res. Bull., 12, 97 (1977).

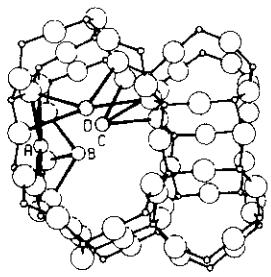
(6) $Ca_{1.9}$[3.8]1.9CO; d + CO; α = 9.43 α = 93.1°
W.J. Mortier, J.J. Pluth, J.V. Smith, Mat. Res. Bull., 12, 103 (1977).

(7) $Na_{15.2}$[4x3.8]; d; C2/m a = 19.32 b = 13.83 c = 11.85 β = 113.5°
[0, 1, 1, 2; 0, -1, 1, 0; 0, -1, -1, 0]
W.J. Mortier, J.J. Pluth, J.V. Smith, Mat. Res. Bull., 12, 241 (1977).

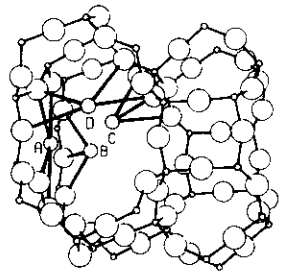
(8) a. $Cu_{1.8}K_{0.2}$[3.9]; d; a = 9.31 α = 92.0°
b. $Cu_{1.8}K_{0.2}$[3.9].xH_2O; h; a = 9.41 α = 95.3°
J.J. Pluth, J.V. Smith, W.J. Mortier, Mat. Res. Bull., 12, 1001 (1977).

*(9) a. $H_{3.2}Ca_{0.2}$[3.6]; d; a = 9.40 α = 93.2°
b. $H_{3.2}Ca_{0.2}$[3.6]; d; a = 9.40 α = 93.3°
W.J. Mortier, G.S.D. King, L. Sengier, J. Phys. Chem., 83, 2263 (1979).

(10) $Ca_{1.4}Sr_{0.3}$[3.8].13H_2O; h; a = 9.42 α = 94.2°
M. Calligaris, G. Nardin, L. Randaccio, P. Comin Chiaramonti, Acta Crystallogr., in press.



DACHIARDITE



DACHIARDITE

Framework DAC = $[Al_xSi_{24-x}O_{48}]$ x = 5 C2/m V = 1374 $\mathring{A}^3$

Extra-framework sites :

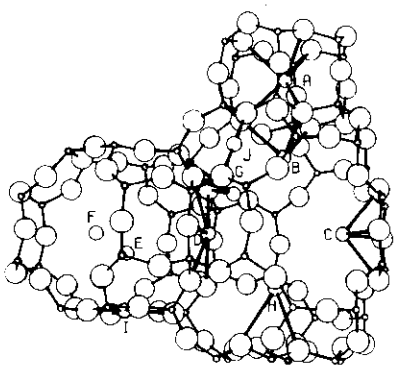
site	type	site symmetry	coordination distances (Å)			
A	III1O	1	3.1	3.1	3.2	3.2
B	IV1O	1	2.7	2.8	2.9	
C	IV1O	1	3.0	3.3	3.3	
D	IV1O	1	3.1	3.1	3.3	3.3

Site occupancies :

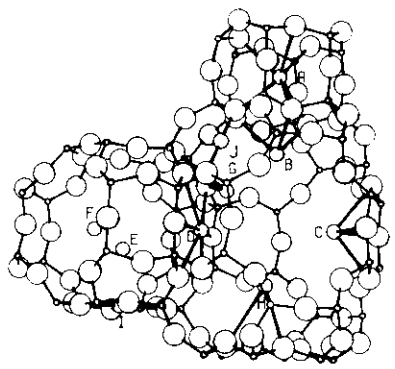
site :	A	B	C	D
(1)	2.4(K,Na,Ca,Mg)	$4H_2O$	$4H_2O$	$4H_2O$

(1) $K_{0.7}Na_{1.1}Ca_{1.6}Mg_{0.1}[5.2].12.7H_2O$; h; B2/m a = 18.7 b = 10.3 c = 7.5 γ = 108°
G. Gottardi, W.M. Meier, Z. Kristallogr., 119, 53 (1963).

EAB



TMA-E (AB)



TMA-E (AB)

Framework EAB = $[Al_xSi_{36-x}O_{72}]$ x = 9 $P6_3/mmc$ V = 2329 $\AA^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)	
A	I	$\bar{6}m2[D_{3h}]$	6x2.97	
B	II8	$3m[C_{3v}]$	3x2.8	
C	IV8	$mm[C_{2v}]$	2x2.6	2x2.8
D	III8	$mm[C_{2v}]$	2x3.2	4x3.2
E	V8	$3m[C_{3v}]$	-	
F	V8	$mm[C_{2v}]$	-	
G	IV8	$m[C_s]$	2x2.7	3.4
H	IV8	$m[C_s]$	2x3.5	
I	II8	$\bar{3}m[D_{3d}]$	6x2.44	
J	II8	$2/m[C_{2h}]$	2x1.81	

Site occupancies :

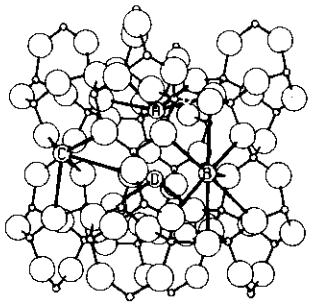
site :	A	B	C	D	E	F	G	H	I	J
(1)a.	-	3.5Na	3Na	$7.3H_2O$	$4.8(N,H_2O)$	$4.2CH_3$	$10.9H_2O$	$6H_2O$	-	-
b.	3.1Ø*	3.7Na 6.7Ø***	$2.4H_2O$***	-	$2.4(N,H_2O)$	7.0CH3***	$10.4H_2O$	-	1.8Ø*	-
c.	4.6Na***	-	$9.6H_2O$***	-	$5.5(N,H_2O)$	-	8.9Ø $10.3H_2O$***	-	-	-

(1) a. $(Me_4N)_2Na_7[9].26H_2O$; h; a = 13.28 c = 15.21

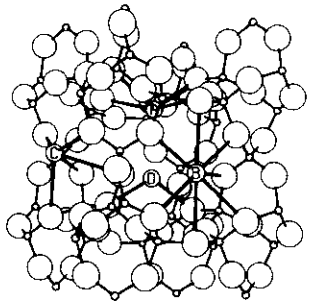
b. $(Me_4N)_yNa_7[9].xH_2O$; d; a = 13.00 c = 15.47

c. $(Me_4N)_yNa_7[9].xH_2O$; d; a = 12.86 c = 15.51

W.M. Meier, M. Groner, J. Solid State Chem., 37, 204 (1981).



EDINGTONITE



EDINGTONITE

Framework EDI = $[Al_xSi_{10-x}O_{20}]$ x = 4 $P2_12_12$ V = 600 $Å^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	III8	2[C_2]	2x2.89 2x2.96 2x3.04
B	III8	1	2.85 2.99 3.17 3.19 3.28 3.33 3.48
C	III8	1	2.94 3.02 3.37 3.45 3.50
D	III8	2[C_2]	2x2.73

Site occupancies :

site :	A	B	C	D
(1)	2Ba	$4H_2O$	$4H_2O$	-
(2)a.	1.3Tl	$2.7Tl^{::}$	-	-
b.	2K	$2K^{::}$, $2H_2O$	$2H_2O$	-
(3)a.	1.2Na, $3.7Na^{::}$	$3.1Na^{::}$, $2.1H_2O^{::}$	-	$0.7H_2O$, $2.0H_2O^{::}$
b.	2.0Rb	2.7Rb, $2.7Rb^{::}$	$3.0H_2O$, 1.4Rb	$2.4H_2O^{:}$, $1.0Rb^{::}$
(4)	2Ba	$4H_2O$	$4H_2O$	-
(5)	2.2K	6.5K, $6.6K^{::}$, $2.1K^{::}$, $2K^{::}$	4.6K, 3.7K, $8ØH^{::}$	$3.3K^{::}$

(1) Ba_2[4].7.$4H_2O$; h; $P\bar{4}2_1m$ a = 9.7 c = 6.6
W.H. Taylor, R. Jackson, Z. Kristallogr., 86, 53 (1933).

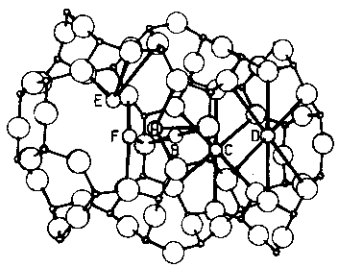
(2) a. Tl_4[4].4.$9H_2O$; h; $P\bar{4}2_1m$ a = 9.94 b = 10.0 c = 6.65
b. K_4[4].3.$6H_2O$; h; $P\bar{4}2_1m$ a = 9.73 b = 10.02 c = 6.68
[both structures described in a tetragonal pseudo-cell : a = 10.0 c = 6.6]
W.H. Taylor, Min. Mag., 24, 208 (1935).

(3) a. Na_5[5].$9H_2O$; h; $P\bar{4}2_1m$ a = 10.06 c = 6.68
b. Rb_{10}[2x5].$13H_2O$; h; I222 a = 9.98 b = 9.98 c = 13.2
[0, 1, 0, 0; 1/2, 0, 1, 0; 0, 0, 0, 2]
C. Baerlocher, R.M. Barrer, Z. Kristallogr., 140, 10 (1974).

$^{:}$(4) Ba_2[4].7.$8H_2O$; h; a = 9.55 b = 9.66 c = 6.52
E. Galli, Acta Crystallogr., B32, 1623 (1976).

(5) $K_{13}(OH)_3$[2x5].$13H_2O$; h; Ccc2 a = 9.90 b = 9.90 c = 13.15
[0, 1, 1, 0; 1/2, -1, 1, 0; 0, 0, 0, 2]
E. Tambuyzer, H.J. Bosmans, Acta Crystallogr., B32, 1714 (1976).

EPI



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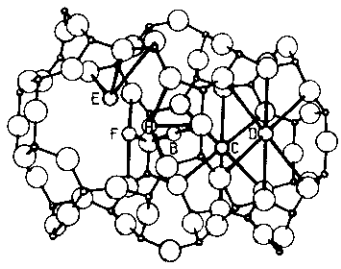


EPISTILBITE

Framework EPI = $[Al_xSi_{24-x}O_{48}]$ x = 6.5 C2/m V = 1350 $Å^3$

Extra-framework sites :

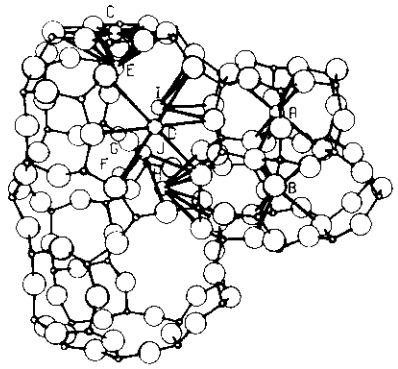
site	type	site symmetry	coordination distances (Å)
A	IV8	m[C_s]	2x2.58 2.60
B	IV8	2/m[C_{2h}]	2x3.03
C	III8	2/m[C_{2h}]	4x3.13 2x3.19
D	III8	2/m[C_{2h}]	2x3.18 4x3.43
E	IV8	1	3.09 3.18 3.46
F	IV8	m[C_s]	2.43 2x2.90

Site occupancies :

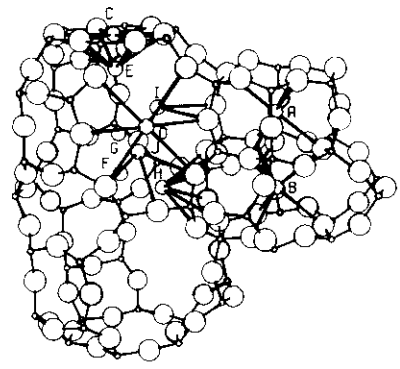
site :	A	B	C	D	E	F
(1)	xCa,Na	xH_2O:::	xH_2O	-	xH_2O	xH_2O
(2)	2.3Ca	0.6H_2O, 2.8H_2O:::	2H_2O	2H_2O	4H_2O, 4H_2O	0.6Ca, 0.5H_2O

:::(1) $Ca_{2.6}Na_{1.1}K_{0.1}$[6.3].15.7H_2O; h; a = 9.08 b = 17.74 c = 10.25 β = 124.9°
A.J. Perrotta, Min. Mag., 36, 480 (1967).

(2) $Ca_{2.7}Na_{0.4}Mg_{0.1}$[6.5].15H_2O; h; C2 a = 9.04 b = 17.75 c = 9.08 β = 111.8°
[0, 1, 0, -1; 0, 0, 1, 0; 1/2, 0, 0, -1]
M. Slaughter, W.T. Kane, Zeit. Kristallogr., 130, 68 (1969).



ERIONITE



ERIONITE

Framework ERI = $[Al_xSi_{36-x}O_{72}]$ x = 9 $P6_3/mmc$ V = 2302 $Å^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)	
A	I	$\bar{3}m[D_{3d}]$	6x2.92	
B	II6	$\bar{6}m2[D_{3h}]$	6x2.98	
C	II8	$\bar{6}m2[D_{3h}]$	3x2.41	3x2.87
D	III8	$2/m[C_{2h}]$	2x3.09	4x3.33
E	II8	$3m[C_{3v}]$	3x2.93	3x3.31
F	V8	$3m[C_{3v}]$	-	
G	V8	$3m[C_{3v}]$	-	
H	IV8	$mm[C_{2v}]$	2x3.22	4x3.41
I	IV8	$m[C_s]$	2x3.19	2x3.43
J	IV8	$m[C_s]$	2x2.87	3.19

Site occupancies :

site :	A	B	C	D	E	F	G	H	I	J
(1)	-	-	-	-	-	-	-	-	-	-
(2)	xCa	xK	xNa	-	-	-	-	-	-	-
(3)	2M	-	-	-	xH_2O	-	-	-	-	-
(4)	2M	-	-	-	xH_2O	-	-	-	-	-
(5)	-	2K	-	0.9M	1.5M	0.7Mg	0.8Ca	$2.0H_2O$	$1.3H_2O$	$2.8H_2O$
(6)	-	2Ca	1.9(Na,Mg)	1.6K	-	-	-	-	-	-

(1) $(Ca,Mg,Na_2,K_2)_{4.5}[9].27H_2O$; h; a = 13.26 c = 15.12
L.W. Staples, J.A. Gard, Miner. Mag., 32, 261 (1959).
[Cations assumed to be randomly distributed on the principal axes of the large cavities.]

(2) $(Ca,Mg,Na_2,K_2)_{4.5}[9].27H_2O$; h; a = 13.26 c = 15.12
O.A. Glonti, N.A. Shishakov, Izv. Akad. Nauk SSSR, Ser. Khim., 1275 (1965).

(3) $Ca_{0.7}Mg_{2.4}Na_{1.3}K_{2.1}[13].xH_2O$; h; a = 13.26 c = 15.12
A. Kawahara, Y. Takano, M. Takabatake, Y. Uratani, Sci. Pap. Coll. Gen. Educ. Univ. Tokyo, 17, 237 (1967).

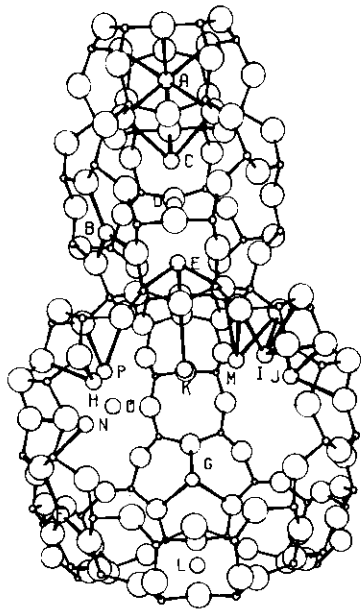
(4) $Ca_{0.7}Mg_{2.4}Na_{1.3}Mg_{0.6}[13].xH_2O$; h; a = 13.26 c = 15.12
A. Kawahara, H. Curien, Bull. Soc. Fr. Mineral. Crystall., 92, 250 (1969).

ERI

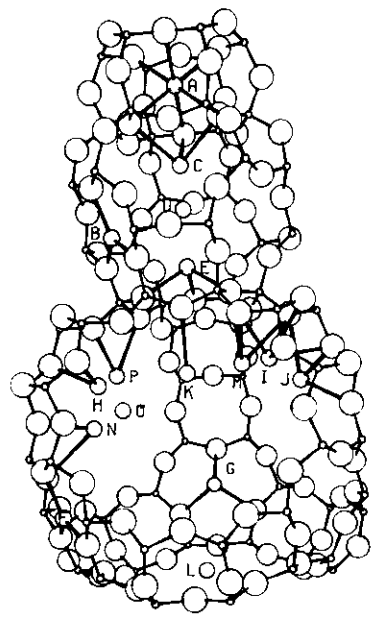
(5) $K_2Na_2Ca_{1.3}Mg_{0.6}[9.3].10.4H_2O$; h;
J.A. Gard, J.M. Tait, Proc. 3rd Int. Conf. Molec. Sieves, J.B. Uytterhoeven, ed., Leuven University Press (Belgium), 94 (1973).

(6) $Mg_{0.7}Na_{0.2}K_{2.0}Ca_{2.4}[9.1].xH_2O$; d; a = 13.25 c = 14.81
J.L. Schlenker, J.J. Pluth, J.V. Smith, Acta Crystallogr., B33, 3265 (1977).

FAU



FAUJASITE



FAUJASITE

Framework FAU = $[Al_xSi_{192-x}O_{384}]$ x = 50-96 Fd3m V = 15500 $\AA^3$

Extra-framework sites :

site[a]	type	site symmetry	coordination distances (Å)
A(I)	I	$\bar{3}m[D_{3d}]$	6x2.8
B	II6	$3m[C_{3v}]$	3x2.2
C(I')	II6	$3m[C_{3v}]$	3x2.6
D(U)	V6	$\bar{4}3m[T_d]$	-
E(II')	II6	$3m[C_{3v}]$	3x2.6
F	II12	$3m[C_{3v}]$	3x2.2
G(II)	II12	$3m[C_{3v}]$	3x2.6
H(III)	IV12	$mm[C_{2v}]$	2x2.7
I(III')	IV12	$m[C_s]$	2x2.7 2x2.7
J	IV12	$m[C_s]$	2.3 2x2.9
K	IV12	$m[C_s]$	2.8
L(V)	V12	$\bar{3}m[D_{3d}]$	-
M	IV12	$m[C_s]$	2x3.1 3.2
N	IV12	1	2.5 3.1
O	V12	$m[C_s]$	-
P	IV12	1	2.6 2.9

(a) The conventional site nomenclature is given in parenthesis.

FAU

Site occupancies :

site :	A	B	C	D	E	F	G
(1)	-	-	(Na,Ca)	-	(Na,Ca)	-	-
(2)	16Na	-	-	-	-	-	32Na
(3)	-	-	16(Na,Ca)	-	$32H_2O$	-	$10.7H_2O$
(4)a.	7.7Na	-	19.5Na	-	-	-	30.3Na
b.	12.0K	-	14.2K	-	-	-	30.0K
c.	16.0Ag	-	10.6Ag	-	-	-	28.3Ag
(5)a.	13.1Ø	-	16.0La	2.9Ø	29.1Ø	-	-
b.	9.2La	-	8.9La	-	-	-	5.5La
(6)	-	-	18Na	-	$32H_2O$	-	-
	+ other sites : $6Ce^{x}$(L)						
(7)	14.2Ca	-	2.6Ca	-	-	-	11.4Ca
(8)	$11.5La^{x}$	-	2.6La	-	1.4Ø	-	1.5La
(9)	-	-	9.7Ca	-	$11.5H_2O$	-	$23.4H_2O^{x}$
	+ other sites : $28.6H_2O$(J); $2.2Ca^{x}$(L)						
(10)	10.6Ni	-	3.1Ni, $5.8H_2O$	-	1.9Ni	1.9Ni	6.4Ni
(11)a.	7.5Ca	-	17.3Ca	-	9.0Ca+10.5Ø	-	17.3Ca
b.	11.2Sr	-	7.0Sr	-	4.2Sr+5.4Ø	-	19.5Sr
c.	10.6Ni	-	3.2Ni+1.9Ni	-	1.9Ni+1.9Ø	-	6.4Ni
(12)a.	-	-	18.0Na	-	$32.0H_2O$	-	$26.0H_2O$
	+ other sites : $5.8Ce^{x}$(L)						
b.	3.4Na	-	11.5Ce	-	16.0Ø	-	10.7Na
c.	-	-	12La	-	$32H_2O$	-	17.0La
	+ other sites : 4La(L)						
d.	-	-	30La	-	32Ø	-	-
(13)	-	-	-	-	-	-	-
(14)	11.7La	-	2.5La	-	-	-	1.4La
(15)a.	32.1Ø	-	13.8La	8.0Ø	24.3Ø	-	13.2La
	+ other sites : $3.4La^{x}$(L)						
b.	5.0La	-	15.2La	3.3Ø	-	-	4.9La
c.	5.2La	-	14.1La	-	-	-	6.3La
(16)	-	-	3.3La	-	28.3Ø	-	$14.2Ø$, $4.4H_2O^{x}$
	+ other sites : $10.3La^{x}$(L)						
(17)	-	-	12.5Ni	-	24Ø	-	2.6Ni
(18)	-	-	12.2Mn	-	27.2Ø	-	5.1Mn
(19)	9.0Na	-	8.0Na, $11.5H_2O$	-	$25.9H_2O^{x}$	-	12.2Na, 11.8Na, $8.0H_2O$, $12.5H_2O^{x}$
	+ other sites : $29.8H_2O$(M); $27.8H_2O^{x}$(K); $17.3H_2O^{x}$(J); $16.3H_2O$(P); $9.6H_2O$(O); $13.4H_2O$(P)						
(20)a.	7.4Na	-	7.3Na	-	-	-	13.1Na
b.	4.5Na	-	3.2Na	-	-	-	9.6Na
c.	1.8Na	-	2.6Na	-	-	-	2.6Na
(21)a.	-	-	13.6K	-	-	-	17.8K
b.	1.3K	-	13.3K	-	-	-	20.0K
c.	7.0K	-	12.0K	-	-	-	24.3K
d.	8.9K	-	7.2K	-	-	-	23.2K
(22)a.	5.8Ce	-	1.9Ce	-	-	-	10Na
b.	1.5Ce	-	8.3Ce	-	24X	-	7Na

(23)a,b,c see (20)

Site occupancies : continued.

site :	A	B	C	D	E	F	G
(24)a.	3.4Cu	-	10.4Cu, 4.6ØH	-	-	-	21Na
b.	2.0Cu	-	13.1Cu	-	9.3NH_3	-	17.4Na
c.	1.7Cu	-	2.5Cu	-	-	-	32.5Na, 6.1N*
	+ 0.6Cu in the center of the large cavity						
(25)a.	-	-	14.7Al	-	32.0ØH	-	-
	+ other sites : 5Na(L)						
b.	-	-	13.4Al	-	15.0ØH	-	-
	+ other sites : 6N(L)						
c.	-	-	14.7Al	-	-	-	-
d.	-	-	7.4Al	-	-	-	-
(26)a.	11.4Ø	9.0Ce	-	-	32Ø	-	21.0Ce
b.	4.2Ce	-	22.7Ce	1.4Ø	-	-	-
	+ other sites : 2.6Ce(L)						
c.	3.2Ce	-	23.7Ce	6.2Ø	-	-	-
(27)a.	8.6K	-	13K	-	-	-	31.6K
b.	7.0Ba	-	4.7Ba	-	-	-	11.4Ba, 3.7Na
c.	3.4Ba	-	4.9Cs	-	2.7Cs	-	19.5Cs, 5.1Na
	+ other sites : 4.2Cs(H)						
d.	5.7Ca	-	5.8Na, 5.8K	-	-	-	12.4Na, 16.1K
(28)a.	6.4K	-	14.1K	-	-	-	26.1K
b.	5.4K	-	18.1K	-	-	-	26.8K
c.	9.4K	-	16.6K	-	-	-	28.9K
d.	9.2K	-	13.6K	-	-	-	25.6K
(29)	-	-	32Na	1.3Te	9.0Na	-	23Na
	+ other sites : 3.7Te(M)						
(30)a.	3.2Cu	-	11.1Cu	-	-	-	20.5Na
b.	2.1Cu	-	12.1Cu	-	9.4NH_3	-	17.8Na
c.	1.9Cu	2.3Cu	-	-	-	-	26.0Na
d.	2.3Cu	-	3.5Cu	-	-	-	22.0Na
e.	1.7Cu	9.9Cu	-	-	-	-	8.0Na
f.	2.1Cu	3.2Cu	-	-	-	-	6.8Na
g.	1.9Cu	-	2.7Cu	-	-	-	5.8Na
(31)	13.3Ca	-	5.0Ca	-	-	-	25.0Ca
(32)a.	11.5Ca	-	-	-	41.0Ø	-	25.4Ø
	+ other sites 8.5Na(M); 23.3Ø(J); 13.3Ø(K)						
b.	12.8Ca	-	-	-	-	-	10.4Ca
c.	1.9Na	-	16.7Na	-	9.8Ø	-	28.8Na
d.	9.3Na	-	16.7Na	-	-	-	26.8Na, 4.5Na
e.	8.6Na	-	11.2Na, 11.7Ø	-	31.7Ø	-	21.7Na, 5.9Ø
	+ other sites : 19.6Na(M); 21.8Ø(K)						
f.	3.8Na*	21.0Na	11.3Na	1.9Ø	-	-	30.8Na
	+ other sites : 7.9Na(M)						
g.	6.1Na	-	18.3Na	2.1Ø	23.3Ø	-	19.0Na, 6.3Na
	+ other sites : 21.3Na(M)						
(33)a.	3.5Ni	-	3.5Ni, 2.5Ni	-	12.5Ø, 1.9Ni	-	23.6Na
b.	4.1Ni	-	2.9Ni, 3.6Ni	-	9.5Ø, 2.1Ni	-	20.0Na
c.	6.9Ni	-	2.5Ni, 3.3Ni	-	5.0Ø, 1.5Ni	-	20.0Na

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Site occupancies : continued.

site :	A	B	C	D	E	F	G
(33)d.	10.2Ni	-	1.3Ni, 1.5Ni	-	-	-	23.2Na
e.	11.7Ni	-	1.1Ni	-	-	-	21.3Na
f.	4.4Ni	-	2.1Ni, 3.6Ni	-	7.5Ø	-	25.9Na
g.	8.8Ni	-	1.7Ni	-	-	-	27.2Na
h.	3.6Ni	-	5.2Ni, 3.1Ni	-	12.0Ø, 4.2Ni	-	12.1Na
i	11.3Ni	-	1.9Ni	-	-	-	20.2Na
(34)a.	2.9Ni	-	4.0Ni	-	11.0NH_3	-	19.1Na
b.	6.6Ni	-	3.8Ni, 1.9Ni	-	5.5N, 3.5N	-	21.0Na
c.	3.3Ni	-	5.2N, 2.5Ni	-	6.0N, 8.0N	-	24.0Na
d.	11.1Ni	-	1.5Ni	-	-	-	22.0Na
e.	9.0Ni	-	2.5Ni	-	-	-	17.0Na
f.	1.7Ni	-	4.8Ni	-	20.0Ø	-	18.0Na
(35)a.	5.4K	-	16.5K	-	-	-	15K
	+ other sites : 5.8H_2O(H)						
b.	-	-	18.6K	-	-	-	14.6K
	+ other sites : 4.7H_2O(H)						
c.	-	-	11.8K	-	-	-	10.2K
d.	-	-	8.4K	-	5.4H_2O	-	7.0K
(36)	-	-	19.7Ca	-	40.4Ø	-	26.7Ø
	+ other sites : 66.8Ø(J)						
(37)a.	1.3Pd	10.6Pd	-	-	-	-	19.0Na
b.	1.7Pd	-	1.5Pd, 4.0Pd	-	-	-	18.0Na
c.	1.7Pd	-	0.8Pd, 4.0Pd	-	-	-	17.0Na
d.	1.9Pd	0.9Pd	0.9Pd	-	-	-	18.0Na
(38)a.	-	-	9.7Ca	-	23.0H_2O	-	23.0H_2O
b.	-	-	9.7Ca	-	30.7H_2O	-	3.1Ca, 11.0H_2O
c.	2.2Na	-	9.6Ca	-	17.7H_2O	-	27.2H_2O
(39)a.	3.2Na	-	3.2Na	-	-	-	3.9Na
b.	3.0Na	-	4.8Na	-	-	-	2.2Na
(40)	-	-	22.7Tl	-	-	-	23.0Tl
(41)a.	5.4Co	-	6.0Co, 7.0H_2O	-	2.7Co	-	21.0Na
b.	9.6Co	-	2.7Co	-	-	-	23.0Na
c.	6.4Co	-	5.8Co, 8.0H_2O	-	3.5Co	-	20.0Na
d.	11.3Co	-	2.3Co	-	-	-	22.0Na
(42)a.	3Na	-	14Na	-	6Na	-	20Na
b.	12Na	-	22Na	-	17Na	-	23Na
c.	20Na	-	11Na	-	12Na	-	30Na
d.	40Na	-	25Na	-	20Na	-	41Na
e.	58Na	-	21Na	-	27Na	-	68Na
f.	78Na	-	66Na	-	16Na	-	110Na
g.	79Na	-	67Na	-	25Na	-	119Na
h.	3Na	-	-	-	20Na	-	11Na
i	8Na	-	11Na	-	25Na	-	12Na
j.	19Na	-	7Na	-	13Na	-	24Na
(43)a.	4.5Al*	-	6.9La	7Ø	-	-	-
b.	-	-	21.1La	2.2Ø	32Ø	-	-

Site occupancies : continued.

site :	A	B	C	D	E	F	G
(44)a.	-	-	6.3Cu	1Ø	26.9Ø	-	22.4Ø
	+ other sites : 11.5H_2O(K); 17.3H_2O*(P); 30.7H_2O(N); 30.7H_2O(N)						
b.	1.5Cu	11.4Cu	2.8Cu	-	1Cu	3.8Cu	1.5Cu, 5.3Ø
	+ other sites : 3.3Cu(P)						
(45)a.	6Na	9.8Pt	-	-	-	-	18Na
b.	8Na	-	3.0Pt	-	-	-	14Na
c.	8Na	-	3.0Pt	-	-	-	14Na
d.	6Na	8.5Pt	-	-	-	-	24Na
e.	5Na	3.8Pt	-	-	-	-	19Na
f.	4Na	-	2.0Pt	-	-	-	9Na
(46)a.	-	-	10.6Ca	-	25.2H_2O	-	6.5Ca
b.	-	-	17.3Na	-	15.4H_2O	-	6.0Ca
c.	-	-	17.3Na	-	13.4H_2O	-	10.2Na
(47)a.	5.0Ø	-	14.9Ø	-	15.5Ø	-	5.7Ø, 9.1Ø
	+ other sites : 21.1Ø(I)						
b.	3.9Ø	-	13.5Ø	-	15.6Ø	-	4.3Ø, 5.8Ø
	+ other sites : 28.6Ø(I)						
c.	0.9Ø	-	15.5Ø	-	14.9Ø	-	8.9Ø, 11.0Ø
	+ other sites : 19.4Ø(I)						
(48)	4.5Ø*	-	13.7Ø	4.6Ø	-	-	15.6Ø, 5.7Ø
	+ other sites : 12.0Ø(L); 29.6Ø(I)						
(49)	3.3Na*	-	11.9Na	-	7.8H_2O	-	1.2Na
	+ other sites : 34.5Na(I)						
(50)a.	4Na	-	17.6Na	-	-	-	32Na
b.	9Na	-	-	-	-	-	9.3Na
(51)a.	6Na	-	4Na	-	-	-	3Na
b.	5Na	-	6Na	-	-	-	7Na
c.	8Na	-	7Na	-	-	-	-
d.	5Na	-	8Na	-	-	-	-
(52)a.	1.9Ag	-	15.7Na	-	15.7H_2O	-	9.7Na
b.	3.9Ag	-	13.5Na, 0.3Ag	-	23.5H_2O	-	8.0Na, 1.8Ag
c.	4.4Ag	-	11.7Na, 1.8Ag	-	18.3H_2O	-	4.0Na, 6.0Ag
(53)a.	-	-	9.7Ca	-	30.7H_2O	-	3.1Ca, 11.4H_2O
b.	-	-	10.9Ca	-	29.0H_2O	-	3.8Ca
c.	5.0Ca	-	17.3Ca	-	26.5H_2O	-	6.6Ca
d.	5.6Ca	-	14.7Ca	-	21.6H_2O	-	6.8Ca
e.	7.8Ca	-	12.0Ca	-	12.8H_2O	-	10.6Ca
f.	13.9Ca	-	4.3Ca	-	3.8H_2O	-	10.4Ca
g.	8.3Ca	-	14.6Ca	-	13.4H_2O	-	8.9Ca
h.	-	-	14.9La	-	23.2H_2O	-	9.4Na
i.	9.8La	-	5.8La	-	-	-	7.5Na
j.	12.6Ca	-	4.0La	-	12.6H_2O	-	16.0Na
(54)a.	-	-	21.5Ca	-	28.5H_2O	-	5.7Ca
b.	-	-	19.3Ca	-	30.5H_2O	-	5.0Ca
c.	1.5Ca	-	18.3Ca	-	28.6H_2O	-	4.6Ca
d.	-	-	19.9Ca	-	22.2H_2O	-	6.5Ca
e.	1.5Ca	-	18.5Ca	-	21.0H_2O	-	6.0Ca

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Site occupancies : continued.

site :	A	B	C	D	E	F	G
(54)f.	-	-	16.0La	-	26.0H_2O	-	4.8Na
g.	6.4Na	-	15.7La	-	29.4H_2O	-	-
h.	10.0Ca	-	12.1Ca	-	26.6H_2O	-	23.0Ca
(55)a.	9Na^{x}	-	10Na, 12H_2O	6H_2O	6H_2O, 7Na	-	1Ce, 9H_2O^{xxx}
	+ other sites : 9H_2O^{xxx}(L); 2H_2O^{xxx}(L); 2.3Ce^{x}(L); 1.7Ce(L)						
b.	10Na^{x}	-	2Ce, 8H_2O	5H_2O	9H_2O	-	7Na, 2Ce, 6H_2O^{xxx}
	+ other sites : 9H_2O^{xxx}(L); 2.8Ce^{x}(L); 2Ce(L)						
c.	2Na, 4Na^{x}	-	3Ce, 6H_2O	7H_2O	7H_2O	7Na	2Ce, 6H_2O^{xxx}
	+ other sites : 7H_2O^{xxx}(L); 7H_2O^{xxx}(L); 2.5Ce^{x}(L); 3.5Ce^{x}(L)						
d.	2Na	-	5.3Ce, 11H_2O	6H_2O	19H_2O	5Na	3.5Ce, 9H_2O^{xxx}
	+ other sites : 9H_2O^{xxx}(L); 1.5Ce^{x}(L); 0.8Ce(L)						
(56)a.	3.6Na	-	11.9Na, 10.3Na 10.4H_2O^{x}	-	26.6H_2O^{x}	-	22.8Na, 5.3H_2O^{x}
	+ other sites : 8H_2O(H); 13.2H_2O(M); 9.5Na(J); 3.8Na(K); 25.6H_2O(P); 20.1H_2O(P); 19.5H_2O(K); 16.4H_2O^{x}(O)						
b.	4.7Na	-	18.3Na, 7.5Na	-	11.0H_2O^{x}, 5.3H_2O^{x}	-	32.3Na, 13.1H_2O^{x}
	+ other sites : 9.9Na(N); 23.5H_2O(I); 9.4Na(K); 24.9H_2O(O); 16.9H_2O(N); 34.5H_2O(N); 21.3H_2O(O)						
(57)a.	4.2Na	-	17.5Na	-	14.5Na, 20.3H_2O^{x}	-	38.8Na
	+ other sites : 13.3Na(J); 19.9H_2O(H); 24.9H_2O^{xxx}(N); 24.5H_2O(N); 13.5H_2O(O)						
b.	-	-	25.3Na, 6.5H_2O	0.8H_2O	25.7Na	-	58.1Na
	+ other sites : 9.0Na(L); 15.7H_2O(K); 34.1H_2O(N); 19.5H_2O(M); 6.7H_2O(H)						
(58)a.	-	-	13.5Na	-	13.5H_2O	-	-
b.	4.6Mn	-	2.8Mn	-	7.2H_2O	-	10.8Mn
c.	-	-	11.8Mn	-	20.2H_2O	-	8.5Mn
(59)a.	-	-	7.3Na	-	-	-	19.0Na
b.	-	-	12.8Na	-	1.4Ru	-	20.1Na
c.	-	-	16.8Na	-	2.4Ru	-	18.9Na
d.	-	-	9.2Na	-	-	-	17.2Na
e.	-	-	17.0Na	-	-	-	17.6Na
(60)a.	12.0Ni	-	9.9Na	-	-	-	24.0Na
b.	11.5Ni	-	9.0Na	-	-	-	24.0Na
c.	5.0Ni	-	17.0Na	-	-	-	24.0Na
(61)	-	-	1.0Cu, 3.1Cu 5.8Cu	-	8.6H_2O	-	4.2Cu, 1.5Cu
	+ other sites : 6.3Cu(P); 1.3Cu(J); 9.0C(H); 14.0C(J^{xxx}); 4.8C(G^{xxx})						
(62)a.	3Na, 5Na^{x}	-	13H_2O, 1Na	3H_2O	11H_2O	-	-
	+ other sites : 5Na^{x}(L); 25Na(I)						
b.	3Na^{x}	-	5Na, 11H_2O, 4Na	3H_2O	6H_2O, 7Na	-	22Na, 4H_2O, 5H_2O^{xxx}
	+ other sites : 3Na^{x}(L); 12Na(I)						
c.	2Na	-	8Na, 15H_2O, 3Na	3H_2O	6H_2O, 4Na	-	25Na, 5H_2O, 6H_2O^{xxx} 5H_2O^{xxx}
	+ other sites : 1Na(L); 5Na(I)						
d.	2Na, 3Na^{x}	-	5Na, 12H_2O, 3Na	-	11H_2O, 5Na	-	24Na, 4H_2O, 6H_2O^{xxx} 5H_2O^{xxx}
	+ other sites : 3Na(L); 3Na(I)						
e.	6Na^{x}	-	7H_2O, 8Na	-	14H_2O, 2Na	24Na, 5H_2O 5H_2O^{xxx}, 3H_2O^{xxx}	-
	+ other sites : 2Na(L); 4Na(I)						

Site occupancies : continued.

site :	A	B	C	D	E	F	G
(62)f.	4Na, 3Na*	-	10Na, $4H_2O$	-	5Na	-	17Na, $5H_2O$, $4H_2O$**** $3H_2O$*****
	+ other sites : 6Na*(L); 8Na(I)						
(63)a.	12Ni	-	9La	-	-	-	16Na
b.	9.5Ni	-	10La	-	-	-	16Na
c.	4Ni	-	16La	-	-	-	14Na
(64)a.	4Na, 9Na*	3Cu	3Na, $6H_2O$, $4H_2O$	-	1Cu, 7Na	-	7Na, $2H_2O$, 3Cu
b.	8Na	6Cu	$5H_2O$	-	$3H_2O$, 15Na	-	2.5Cu, 7Na
c.	1Ce	4Na	7Ce, $21H_2O$	$5H_2O$	$10H_2O$, 1Na, $1H_2O$	-	1.3Ce, 19Na, $5H_2O$
d.	1.6Ce	9Na	8Ce, $13H_2O$	$4H_2O$	$11H_2O$, $9H_2O$	-	23Na, $9H_2O$
e.	2Ce, 2.5Ce*, 3Na*	-	6Na, 6.5Na, $2H_2O$, $7H_2O$	$3H_2O$	-	-	2Cu, 1Cu, 3Ce
f.	2.3Ce, 2.5Ce*, 4Na*	-	5Na, 7Ce, $9H_2O$	-	$6H_2O$	-	1.3Cu, 1.3Cu, 2Ce
(65)a.	7.5Fe	-	2.9Fe	-	-	-	16Na
b.	8.3Fe	-	10.6Na	-	-	-	5.7Fe
c.	2.7Fe	-	5.1Fe, 15Na	-	-	-	16Na
d.	-	-	7.4Fe	-	-	-	18Na
(66)a.	-	-	4.2Cr, 22Na	-	12.2Ø	-	32Na
b.	-	-	3.8Cr, 9Na	-	-	-	28Na
c.	7.4Na	-	3.8Cr, 3.4Na	-	-	-	30Na
d.	9.1Na	-	3.8Cr, 4.1Na	-	-	-	27Na
e.	-	-	8.0Na	-	-	-	28Na
(67)a.	12.8Ag	-	13.1Ag	-	5.4Ag	-	19.5Ag
b.	14.7Ag	-	15.7Ag	-	9.3Ag	-	21.4Ag
c.	14.7Ag	-	21.1Ag	-	9.0Ag	-	20.5Ag
	+ other sites : 10.5Ag(I); 3.9Ag(I)						
d.	15.2Ag	-	25.0Ag	-	8.0Ag	-	24.6Ag
	+ other sites : 19.0Ag(I)						
e.	11.5Ag	-	12.5Ag	-	2Ag, $30H_2O$	-	14.1Ag, 6.7Ag
(68)a.	10.2Ag	-	5.8Ag	-	2.4Ag	-	18.5Ag
b.	13.1Ag	-	13.2Ag	-	4.8Ag	-	19.7Ag
c.	5.4Ag	-	25.7Ag	-	5.8Ag, 2.2Ag	-	15.8Ag
d.	10.7Ag	-	24.6Ag	-	13.4Ag	-	13.4Ag
e.	4.4Ag	-	28.0Ag	-	15.5Ag	-	7.5Ag
f.	7.8Ag, 3.8Ag	-	21.1Ag	-	4.5Ag, 1.6Ag	-	17.9Ag
(69)a.	0.6Na	-	7.7Na	-	-	-	6.4Na
	+ other sites : 4.8Pd*(L)						
b.	1.4Na	9.2Pd	-	-	-	-	18.9Na
c.	2.2Na	12.0Pd	-	-	-	-	14.7Na

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(8) La_{19}[57]; d; a = 24.71
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(9) Ca_{27}[57].xH_2O; h; a = 24.62
J.M. Bennett, J.V. Smith, Mat. Res. Bull., 3, 933 (1968).

(10) $Ni_{27}Ca_4$[58].xH_2O; h; a = 24.41
D.H. Olson, J. Phys. Chem., 72, 4366 (1968).

(11) a. Ca_x[86]; d;
b. Sr_x[86]; d;
c. Ni_x[59]; d;
D.H. Olson, J. Phys. Chem., 72, 1400 (1968).

(12) a. $Ce_{12}(Ca,Mg)_{7.6}Na_{7.8}$[59].270$H_2O$; h; a = 24.69
b. $Ce_{12}(Ca,Mg)_{7.6}Na_{7.8}$[59]; d; a = 24.69
c. $La_{29.1}Na_{0.4}$[86.8].270H_2O; h; a = 25.09
d. $La_{29.1}Na_{0.4}$[86.8].xH_2O; d+H_2O; a = 24.98
D.H. Olson, G.T. Kokotailo, J.F. Charnell, J. Coll. Interf. Sci., 28, 305 (1968).

(13) H_{59}[59]; d; a = 24.76
D.H. Olson, E. Dempsey, J. Catal., 13, 221 (1969).

(14) La_{19}[57]; d; a = 24.71
J.M. Bennett, J.V. Smith, Mat. Res. Bull., 4, 7 (1969).

(15) a. $La_{26.4}Na_{4.6}$[82].260H_2O; h; a = 25.05
b. $La_{26.4}Na_{4.6}$[82]; d; a = 25.05
c. $La_{26.4}Na_{4.6}$[82]; d; a = 25.05
J.M. Bennett, J.V. Smith, Mat. Res. Bull., 4, 77 (1969).

(16) La_{19}[57].xH_2O; h; a = 24.69
J.M. Bennett, J.V. Smith, Mat. Res. Bull., 4, 343 (1969).

(17) $Ni_{28.5}$[57].24-32$C_6H_4Cl_2$; d+$C_6H_4Cl_2$; a = 24.45
H.D. Simpson, H. Steinfink, J. Amer. Chem. Soc., 91, 6225 (1969).

(18) $Mn_{28.5}$[57].24C_4H_9Cl; d+C_4H_9Cl; a = 24.37
H.D. Simpson, H. Steinfink, J. Amer. Chem. Soc., 91, 6229 (1969).

(19) Na_{88}[88].220H_2O; h; Fd3 a = 25.028
D.H. Olson, J. Phys. Chem., 74, 2758 (1970).

(20) a. $Na_{27}H_{29}$[56]; d; a = 24.75
b. $Na_{14}H_{42}$[56]; d; a = 24.71
c. Na_2H_{54}[56]; d; a = 24.67
P. Gallezot, B. Imelik, C.R. Acad. Sc. Paris, ser. B, 271, 912 (1970).

(21) a. K_{48}[48].243H_2O; h; a = 24.69
b. K_{55}[55].241H_2O; h; a = 24.73
c. K_{70}[70].247H_2O; h; a = 24.92

d. $K_{87}[87].258H_2O$; h; a = 25.12

W.J. Mortier, H.J. Bosmans, J. Phys. Chem., 75, 3327 (1971).

(22) a. $Ce_8Na_8H_{23}[56]$; d; a = 24.76

b. $Ce_8Na_8H_{23}[56]$; d+air; a = 24.72

P. Gallezot, B. Imelik, J. Chim. Phys. Physicochim. Biol., 68, 34 (1971).

(23) a,b,c, see (20)

P. Gallezot, B. Imelik, J. Chim. Phys. Physicochim. Biol., 68, 816 (1971).

(24) a. $Cu_{16}Na_{24}[56]$; d;

b. $Cu_{16}Na_{24}[56]$; d+NH_3;

c. $Cu_{16}Na_{24}[56]$; d+Py;

P. Gallezot, Y. Ben Taarit, B. Imelik, C.R. Acad. Sci. Paris, ser. C, 272, 261 (1971).

(25) a. $Na_9H_{44}[53]$; d; a = 24.56

b. $(NH_4,H)_9Na_1[53].xH_2O$; d in air; a = 24.59

c. $Na_1[53]$; b+d; a = 24.31

d. $Na_1[53]$; c+2x(NH_4SO_4+d); a = 24.24

P.K. Maher, F.D. Hunter, J. Scherzer, Adv. Chem. Ser., 101, 266 (1971).

(26) a. $Na_1Ce_{26}[88].xH_2O$; h; a = 25.10

b. $Na_1Ce_{26}[88]$; d + air; a = 24.94

c. $Na_1Ce_{26}[88]$; d + air; a = 24.86

F.D. Hunter, J. Scherzer, J. Catalysis, 20, 246 (1971).

(27) a. $K_{53}[53]$; d; a = 24.87

b. $Ba_{36}Na_{16}[52]$; d; a = 24.85

c. $Cs_{31}Na_9Ba_2K_2Ca_1[50]$; d; a = 24.71

d. $K_{17}Na_{11}Ca_5[52]$; d; a = 24.71

J.J. Pluth, Ph.D. thesis, University of Washington 1971, University Microfilms, no. 71-28459, Ann Arbor, Michigan, U.S.A.

(28) a. $K_{48}[48]$; d; a = 24.78

b. $K_{55}[55]$; d; a = 24.82

c. $K_{70}[70]$; d; a = 24.97

d. $K_{87}[87]$; d; a = 25.08

W.J. Mortier, H.J. Bosmans, J.B. Uytterhoeven, J. Phys. Chem., 76, 650 (1972).

(29) $Na_{86}[86]$.11% Te; d + Te + H_2; a = 24.76

D.H. Olson, R.J. Mikovsky, G.F. Shipman, E. Dempsey, J. Catalysis, 24, 161 (1972).

(30) a. $Cu_{16}Na_{24}[56]$; d; a = 24.66

b. $Cu_{16}Na_{24}[56].xNH_3$; d+NH_3; a = 24.63

c. $Cu_{16}Na_{24}[56].xC_5H_5N$; d + C_5H_5N; a = 24.66

d. $Cu_{16}Na_{24}[56].xC_{10}H_8$; d + $C_{10}H_8$; a = 24.70

e. $Cu_{12}Na_5H_{27}[56]$; d; a = 24.61

f. $Cu_{12}Na_5H_{27}[56].xC_{10}H_8$; d + $C_{10}H_8$; a = 24.69

g. $Cu_{12}Na_5H_{27}[56].xC_4H_8$; d + C_4H_8; a = 24.69

P. Gallezot, Y. Ben Taarit, B. Imelik, J. Catalysis, 26, 295 (1972).

(31) $Ca_{40}[80]$; d; a = 24.97

J.J. Pluth, J.V. Smith, Mat. Res. Bull., 7, 1311 (1972).

(32) a. $(Na_2,Ca)_{14.4}[58].xH_2O$; ; a = 24.68

b. $(Na_2,Ca)_{14.4}[58]$; ; a = 24.57

c. $Na_{58}[58].xH_2O$; h; a = 24.74

d. $Na_{58}[58]$; d; a = 24.79

e. $Na_{81}[81].xH_2O$; h; a = 24.92

f. $Na_{81}[81]$; d; a = 24.92

g. $Na_{81}[81].xH_2O$; h; a = 24.99

T. Hseu, Ph.D. Thesis, University of Washington 1972, University Microfilms, no. 73-13835, Ann Arbor, Michigan, U.S.A.

(33) a. $Ni_{14}Na_{23}H_5[56]$; d; a = 24.63

b. $Ni_{14}Na_{23}H_5[56]$; d; a = 24.62

c. $Ni_{14}Na_{23}H_5[56]$; d; a = 24.57

d. $Ni_{14}Na_{23}H_5[56]$; d; a = 24.51

e. $Ni_{14}Na_{23}H_5[56]$; d; a = 24.47

f. $Ni_{10}Na_{31}H_5[56]$; d; a = 24.67

g. $Ni_{10}Na_{31}H_5[56]$; d; a = 24.59

h. $Ni_{19}Na_{31}H_3[56]$; d; a = 24.56

i. $Ni_{19}Na_{31}H_3[56]$; d; a = 24.40

P. Gallezot, B. Imelik, J. Phys. Chem., 77, 652 (1973).

(34) a. $Ni_{14}Na_{23}H_5[56].xNH_3$; d + NH_3; a = 24.66

b. $Ni_{14}Na_{23}H_5[56].xNO$; d + NO; a = 24.58

c. $Ni_{14}Na_{23}H_5[56].xNO$; d + NO; a = 24.62

d. $Ni_{14}Na_{23}H_5[56].xC_5H_5N$; d + C_5H_5N; a = 24.48

e. $Ni_{14}Na_{23}H_5[56].xC_5H_5N$; d + C_5H_5N; a = 24.53

f. $Ni_{14}Na_{23}H_5[56].xC_5H_5N$; d + C_5H_5N; a = 24.66

P. Gallezot, Y. Ben Taarit, B. Imelik, J. Phys. Chem., 77, 2556 (1973).

(35) a. $(C_3H_7NH_3)_{19}K_{36}[55].101H_2O$; h; a = 24.75

b. $(C_2H_5NH_3)_{23}K_{31}[55].111H_2O$; h; a = 24.75

c. $(CH_3NH_3)_{28}K_{27}[55].124H_2O$; h; a = 24.74

d. $(NH_4)_{34}K_{15}[55].190H_2O$; h; a = 24.74

W.J. Mortier, M.L. Costenoble, J.B. Uytterhoeven, J. Phys. Chem., 77, 2880 (1973).

(36) $Ca_{40}[80].xH_2O$; h; a = 24.84

J.J. Pluth, J.V. Smith, Mat. Res. Bull., 8, 459 (1973).

(37) a. $Pd_{13}Na_{20}H_{12}[56]$; d; a = 24.66

b. $Pd_{13}Na_{20}H_{12}[56]$; d + H_2; a = 24.71

c. $Pd_{13}Na_{20}H_{12}[56]$; d + H_2; a = 24.71

d. $Pd_{13}Na_{20}H_{12}[56]$; d + H_2; a = 24.71

P. Gallezot, B. Imelik, Adv. Chem. Ser., 121, 66 (1973).

(38) a. $Ca_{27}Na_3[57].252H_2O$; h;

b. $Ca_{27}Na_3[57].252H_2O$; d + air;

c. $Ca_{27}Na_3[57].232H_2O$; h;

M.L. Costenoble and W.J. Mortier, Proc. Third Int. Conf. Molecular Sieves, 120 (1973).

(39) a. $Na_9H_{46}[55]$; d; a = 24.67

b. $Na_4H_{23}[27]$; d; a = 24.53

P. Gallezot, R. Beaumont, D. Barthomeuf, J. Phys. Chem., 78, 1550 (1974).

(40) $Tl_{88}[88].xH_2O$; h; a = 25.09

J.J. De Boer, I.E. Maxwell, J. Phys. Chem., 78, 2395 (1974).

(41) a. $Co_{19}Na_{18}[56]$; d; a = 24.65

b. $Co_{19}Na_{18}[56]$; d; a = 24.55

c. $Co_{14}Na_{25}[56]$; d; a = 24.55

d. $Co_{14}Na_{25}[56]$; d; a = 24.40

P. Gallezot, B. Imelik, J. Chim. Phys., 71, 155 (1974).

(42) a. $Na_{70}[78].xH_2O$; h;

b. $Na_{72}Ag_6[78].xH_2O$; h;

c. $Na_{69}Ag_9[78].xH_2O$; h;

d. $Na_{55}Ag_{23}[78].xH_2O$; h;
e. $Na_{44}Ag_{34}[78].xH_2O$; h;
f. $Na_{12}Ag_{66}[78].xH_2O$; h;
g. $Ag_{78}[78].xH_2O$; h;
h. $Na_{52}[55].xH_2O$; h;
i. $Na_{38}Ag_{17}[55].xH_2O$; h;
j. $Na_{27}Ag_{28}[55].xH_2O$; h;
L.P. Aldridge, C.G. Pope, J. Inorg. Nucl. Chem., 36, 2097 (1974).
[The site populations in the table are given in electron density equivalents of Na].

(43) a. $H_{46}Na_2La_5[62].xH_2O$; d + H_2O; a = 24.49
b. $Na_2La_{20}[62].xH_2O$; d + H_2O; a = 24.75
J. Scherzer, J.L. Bass, F.D. Hunter, J. Phys. Chem., 79, 1194 (1975).

(44) a. $Cu_{28}[56].xH_2O$; h; a = 24.71
b. $Cu_{28}[56]$; d; a = 24.64
I.E. Maxwell, J.J. de Boer, J. Phys. Chem., 79, 1874 (1975).

(45) a. $Pt_{10}Na_{17}H_{19}[56]$; d; a = 24.68
b. $Pt_{10}Na_{17}H_{19}[56]$; d + H_2 + d; a = 24.70
c. $Pt_{10}Na_{17}H_{19}[56]$; d + H_2 + d; a = 24.50
d. $Pt_{10}Na_{17}H_{19}[56]$; d; a = 24.68
e. $Pt_{10}Na_{17}H_{19}[56]$; d; a = 24.71
f. $Pt_{10}Na_{17}H_{19}[56]$; d + H_2 + d; a = 24.74
P. Gallezot, A. Alarcon-Diaz, J.-A. Dalmon, A.J. Renouprez, B. Imelik, J. Catalysis, 39, 334 (1975).

(46) a. $K_6Ca_{25}[57].235H_2O$; h; a = 24.72
b. $Na_{18}Ca_{19}[57].242H_2O$; h; a = 24.68
c. $Na_{57}[57].268H_2O$; h; 24.70
M.L. Costenoble, W.J. Mortier and J.B. Uytterhoeven, J.C.S. Faraday Trans. I, 72, 1877 (1976).

(47) a. $Cu_7Na_{29}H_{13}[56].250H_2O$; h; a = 24.70
b. $Cu_{12}Na_{21}H_{11}[56].250H_2O$; h; a = 24.70
c. $Cu_{15}Na_{16}H_{10}[56].250H_2O$; h; a = 24.68
J. Marti, J. Soria, F.H. Cano, J. Phys. Chem., 80, 1776 (1976).
[The site populations in the table are given in electron density equivalents of oxygen].

(48) $Ce_{4.7}Na_{26.3}H_{15.7}[56].250H_2O$; h; a = 24.72
J. Marti, J. Soria, F.H. Cano, Anales de Fisica, 72, 130 (1976).
[The site populations in the table are given in electron density equivalents of oxygen].

(49) $Na_{57}[57].xH_2O$; h; a = 24.66
J. Marti, J. Soria, F.H. Cano, J. Coll. Interf. Sci., 40, 82 (1977).

(50) a. $Na_{53}Ca[55]$; d;
b. $Na_{13}CaH_{40}[55]$; d;
Z. Jirak, S. Vratislav, J. Zajicek, V. Bosacek, J. Catalysis, 49, 112 (1977).
[Several hydrogen positions for sample (b) are given in the paper].

(51) a. $Na_{10}H_{46}[56].8Mo(CO)_6$; d + $Mo(CO)_6$; a = 24.75
b. $Na_{10}H_{46}[56].4Re_2(CO)_{10}$; d + $Re_2(CO)_{10}$; a = 24.75
c. $Na_{10}H_{46}[56].4Re_2(CO)_x$; d + $Re_2(CO)_{10}$ + d; a = 24.73
d. $Na_{10}H_{46}[56].3Ru_3(CO)_{12}$; d + $Ru_3(CO)_{12}$; a = 24.70
P. Gallezot, G. Coudurier, M. Primet, B. Imelik, A.C.S. Symp. Ser., 40, 144 (1977).

(52) a. $Na_{53}Ag_2[55].xH_2O$; h; a = 24.69
b. $Na_{48}Ag_7[55].xH_2O$; h; a = 24.69
c. $Na_{41}Ag_{14}[55].xH_2O$; h; a = 24.69
M.L. Costenoble, A. Maes, J.C.S. Faraday Trans. I, 74, 131 (1978).

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(53) a. $Na_3Ca_{27}[57].252H_2O$; h; a = 24.67
b. $Na_3Ca_{27}[57].92H_2O$; d; a = 24.64
c. $Na_3Ca_{27}[57].28H_2O$; d; a = 24.74
d. $Na_3Ca_{27}[57].20H_2O$; d; a = 24.74
e. $Na_3Ca_{27}[57].11H_2O$; d; a = 24.76
f. $Na_3Ca_{27}[57]$; d; a = 24.76
g. $Na_3Ca_{27}[57].11H_2O$; d; a = 24.76
h. $Na_3La_{16}H_5[57].13H_2O$; d; a = 24.87
i. $Na_3La_{16}H_5[57]$; d; a = 24.79
j. $Na_3Ca_{41}[86].8H_2O$; d; a = 24.97
M.L. Costenoble, W.J. Mortier, J.B. Uytterhoeven, J.C.S. Faraday Trans. I, 74, 466 (1978).

(54) a. $Na_3Ca_{27}[57].28H_2O$; d; a = 24.71
b. $Na_3Ca_{27}[57].20H_2O$; d; a = 24.72
c. $Na_3Ca_{27}[57].11H_2O$; d; a = 24.71
d. $Na_3Ca_{27}[57]$; d; a = 24.71
e. $Na_3Ca_{27}[57].11H_2O$; d; a = 24.74
f. $Na_3La_{16}H_5[57].13H_2O$; d; a = 24.87
g. $Na_3La_{16}H_5[57]$; d; a = 24.86
h. $Na_3Ca_{41}[86].8H_2O$; d; a = 24.98
M.L. Costenoble, W.J. Mortier, J.B. Uytterhoeven, J.C.S. Faraday Trans. I, 74, 477 (1978).

(55) a. $Ce_5Na_{26}H_{17}[56].250H_2O$; h; a = 24.72
b. $Ce_{10.5}Na_{5.0}H_{19.6}[56].250H_2O$; h; a = 24.74
c. $Ce_{12.7}Na_{2.8}H_{15.2}[56].250H_2O$; h; a = 24.75
d. $Ce_{14.2}Na_{15.1}[56].250H_2O$; h; a = 24.76
J. Marti, J. Soria, F.H. Cano, J. Coll. Interf. Sci., 67, 266 (1978).

(56) a. $Na_{81}[81].240H_2O$; h; a = 24.89
b. $Na_{81}[81].240H_2O$; h; a = 24.89
Yu.I. Smolin, Yu.F. Shepelev, I.K. Butikova, S.P. Zhdanov, N.N. Samulevich, Kristallografiya, 24, 461 (1979).

(57) a. $Na_{40.5}Nd_{13.8}[81].xH_2O$; h; a = 24.91
b. $Na_{20.3}Nd_{20.2}[81].xH_2O$; h; a = 24.95
Yu.F. Shepelev, Yu.I. Smolin, I.K. Butikova, N.I. Kozlova, Kristallografiya, 24, 469 (1979).

(58) a. $Mn_{19.3}Na_{17.4}[56].256H_2O$; h; a = 24.68
b. $Mn_{19.3}Na_{17.4}[56].5.1H_2O$; d; a = 24.72
c. $Mn_{19.3}Na_{17.4}[56].5.1H_2O$; d; a = 24.73
J.R. Pearce, W.J. Mortier, J.B. Uytterhoeven, J.C.S. Faraday Trans. I, 75, 898 (1979).

(59) a. $Ru_8Na_{34}[56]$; d; a = 24.81
b. $Ru_8Na_{34}[56]$; d + H_2; a = 24.83
c. $Ru_8Na_{34}[56]$; d + H_2; a = 24.76
d. $Ru_8Na_{34}[56]$; d + H_2 + O_2; a = 24.82
e. $Ru_8Na_{34}[56]$; d + H_2 + O_2 + H_2; a = 24.81
J.R. Pearce, W.J. Mortier, J.B. Uytterhoeven, J.C.S. Faraday Trans. I, 75, 1395 (1979).

(60) a. $Ni_{17}Pt_{0.5}Na_{40}H_{11}[86]$; d; a = 24.54
b. $Ni_{17}Pt_{0.5}Na_{40}H_{11}[86]$; d + H_2; a = 24.58
c. $Ni_{17}Pt_{0.5}Na_{40}H_{11}[86]$; d + H_2; a = 24.64
J. Jeanjean, D. Delafosse, P. Gallezot, J. Phys. Chem., 83, 2761 (1979).

(61) Cu_{28}[56].xC_4H_6; d + C_4H_6; a = 24.72
I.E. Maxwell, J.J. de Boer, R.S. Downing, J. Catalysis, 61, 493 (1980).

(62) a. Na_{57}[57].xH_2O; d; a = 24.66
b. Na_{57}[57].xH_2O; d(298K); a = 24.79
c. Na_{57}[57].xH_2O; d(403K); a = 24.76
d. Na_{57}[57].xH_2O; d(423K); a = 24.75
e. Na_{57}[57].xH_2O; d(473K); a = 24.80
f. Na_{57}[57]; d(773K); a = 24.79
J.A. Rubio, J. Soria, F.H. Cano, J. Colloid Interf. Sci., 73, 312 (1980).

(63) a. $Ni_{14}La_{15}Na_{12}$[85]; d; a = 24.91
b. $Ni_{14}La_{15}Na_{12}$[85]; d + H_2(693K); a = 24.95
c. $Ni_{14}La_{15}Na_{12}$[85]; d + H_2(873K); a = 24.80
M. Briend-Faure, J. Jeanjean, D. Delafosse, P. Gallezot, J. Phys. Chem., 84, 875 (1980).

(64) a. $Cu_{15.3}Na_{18.8}H_{7.4}$[57]; d;
b. $Cu_{15.3}Na_{18.8}H_{7.4}$[57]; d;
c. $Ce_{10.1}Na_{20.0}H_{6.8}$[57]; d;
d. $Ce_{10.1}Na_{20.0}H_{6.8}$[57]; d;
e. $Ce_{11.4}Cu_{4.8}Na_{9.1}H_4$[57]; d; a = 24.75
f. $Ce_{11.4}Cu_{4.8}Na_{9.1}H_4$[57]; d; a = 24.75
R. Cid, J.C. Conera, J. Marti, L. Mercader, J. Soria, Proc. Fifth Int. Conf. Zeolites, L.V. Rees, ed., Heyden (London 1980), p. 714.

(65) a. $Fe_{13}Na_{24}H_6$[56]; d; a = 24.61
b. $Fe_{13}Na_{24}H_6$[56]; d + H_2; a = 24.60
c. $Fe_{13}Na_{24}H_6$[56]; d + O_2; a = 24.78
d. $Fe_{13}Na_{24}H_6$[56]; d + O_2 + d + H_2; a = 24.72
J.R. Pearce, W.J. Mortier, J.B. Uytterhoeven, J.H. Lunsford, J.C.S. Faraday Trans. I, 77, 937 (1981).

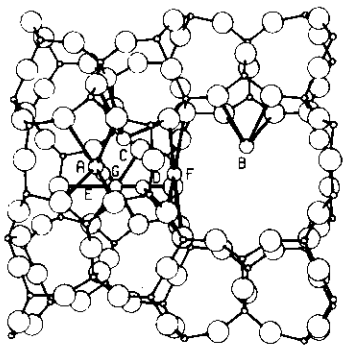
(66) a. $Cr_{4.2}Na_{73.4}$[86]; d; a = 25.05
b. $Cr_{3.8}Na_{44.3}$[56]; d; a = 24.77
c. $Cr_{3.8}Na_{44.3}$[56]; d; a = 24.77
d. $Cr_{3.8}Na_{44.3}$[56]; d + H_2 + d; a = 24.77
e. $Cr_{3.8}Na_{44.3}$[56].xNO; d + NO + d; a = 24.78
J.R. Pearce, W.J. Mortier, J.C.S. Faraday Trans. I, 76, 0000 (1981).

(67) a. $Ag_{55.5}$[55.5]; d + O_2 + d; a = 24.82
b. $Ag_{69.8}$[69.8]; d + O_2 + d; a = 24.96
c. $Ag_{82}Na_4$[86]; d + O_2 + d; a = 25.06
d. Ag_{101}[101]; d + O_2 + d; a = 25.11
e. $Ag_{82}Na_4$[86].264H_2O; h; a = 25.01
L.R. Gellens, W.J. Mortier, J.B. Uytterhoeven, Zeolites, 1, 11 (1981).

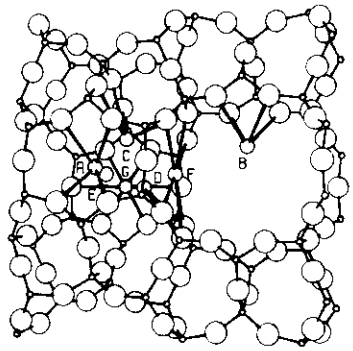
(68) a. $Ag_{55.5}$[55.5]; d; a = 24.82
b. $Ag_{55.5}$[55.5]; d + O_2; a = 24.85
c. $Ag_{55.5}$[55.5]; d + O_2 + d + H_2 + d; a = 24.62
d. $Ag_{55.5}$[55.5]; d + O_2 + d + H_2 + d; a = 24.69
e. $Ag_{55.5}$[55.5]; d + O_2 + d + H_2 + d + O_2 + d; a = 24.67
f. $Ag_{55.5}$[55.5]; d + O_2 + d + H_2 + d + O_2; a = 24.78
L.R. Gellens, W.J. Mortier, J.B. Uytterhoeven, Zeolites, 1, 85 (1981).

(69) a. $Pd_{13.7}Na_{9.3}H_{19.2}$[56]; d; a = 24.71
b. $Pd_{13.7}Na_{9.3}H_{19.2}$[56]; d; a = 24.75
c. $Pd_{13.7}Na_{9.3}H_{19.2}$[56]; d; a = 24.69
G. Bergeret, P. Gallezot, B. Imelik, J. Phys. Chem., 85, 411 (1981).

FER



FERRIERITE



FERRIERITE

Framework FER = $[Al_xSi_{36-x}O_{72}]$ x = 5.5 Immm V = 2028 $\AA^3$

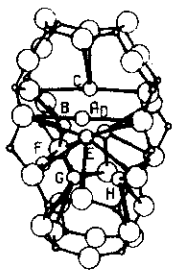
Extra-framework sites :

site	type	site symmetry	coordination distances ($\AA$)
A	II8	mm[C_{2v}]	4x2.94
B	IV10	mm[C_{2v}]	4x3.06
C	IV8	m[C_s]	3.31 3.25 2x3.38
D	IV8	m[C_s]	3.15 2x3.25
E	V8	mmm[D_{2h}]	-
F	III10	mm[C_{2v}]	2x3.12 4x3.26
G	II8	mmm[D_{2h}]	4x2.33 2x3.01

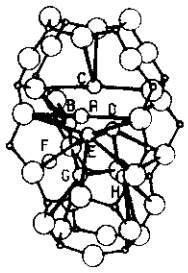
Site occupancies :

site :	A	B	C	D	E	F	G
(1)	$4H_2O$	0.95Na	$4H_2O$	$4H_2O$	2Mg	-	-

(1) $Na_{1.5}Mg_2[5.5].18H_2O$; h; a = 19.16 b = 14.13 c = 7.49
P.A. Vaughan, Acta Crystallogr., 21, 983 (1966).



GISMONDINE



GISMONDINE

Framework GIS = $[Al_xSi_{16-x}O_{32}]$ x = 8 $P2_1/a$ V = 1046 $Å^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)				
A	III8	$\bar{1}[C_i]$	2x2.82				
B	III8	1	2.44	2.55	3.09	3.32	
C	IV8	1	2.85	2.99	3.11	3.26	
D	IV8	1	2.85	2.86	3.04	3.11	
E	III8	1	3.09	3.15	3.21	3.26	3.33
F	III8	1	2.90	2.95			
G	IV8	1	2.97	3.13	3.35	3.35	
H	IV8	1	3.00	3.13	3.21	3.35	

Site occupancies :

site :	A	B	C	D	E	F	G	H
(1)	-	4Ca	$4H_2O$	$4H_2O$	$4H_2O$	$2H_2O$	$2H_2O$	-
(2)	-	8C:::	8C:::	4N:::	-	-	-	-
(3)	-	3.7Ca	$3.5H_2O$	$4H_2O$	$3.8H_2O$	$2.4H_2O$	$1.9H_2O$	$1.6H_2O$
(4)	5.6Ø:, 4Ø:	-	-	-	1.4Ø:::, 3.4Ø	-	2.6Ø	-
(5)	-	$4H_2O$	-	$4H_2O$	4Na	4K:::	$2H_2O$, $1.1H_2O$:::	-

(1) $Ca_4[8].16H_2O$; h; $P2_1/c$ a = 10.02 b = 10.62 c = 9.84 β = 92.4°
[0, 0, 0, 1; 0, 1, 0, 0; 0, 0, 1, 0]
K. Fischer, Amer. Mineral., 48, 664 (1963).

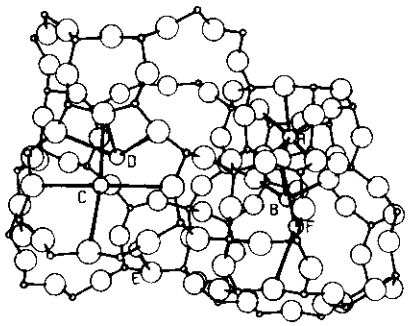
(2) $(CH_3)_{16}N_4[4].xH_2O$; h; $I4_1/amd$ a = 10.46 c = 9.73
[0, 1, 0, 0; 0, 0, 1, 0; 0, 0, 0, -1]
Ch.Baerlocher, W.M. Meier, Helv. Chim. Acta, 53, 1285 (1970).

:(3) $Ca_{3.7}[7.2].17.2H_2O$; h; a = 9.84 b = 10.02 c = 10.62 γ = 92.4°
K.F. Fischer, V. Schramm, Adv. Chem. Ser., 101, 250 (1971).

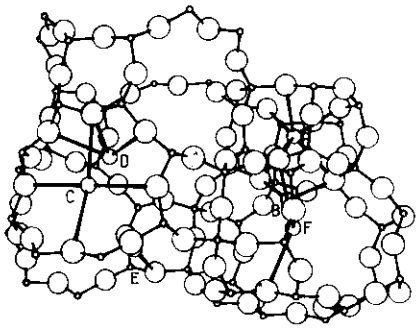
(4) $Na_6[6].12H_2O$; h; $I\bar{4}$ a = 10.04 c = 10.04
[1/2, 1, 0, 0; 1/4, 0, 1, 0; 3/8, 0, 0, 1]
Ch. Baerlocher, W.M. Meier, Zeit. Kristallogr., 135, 339 (1972).

(5) $K_4Na_4[8].10H_2O$; h; I2 a = 10.23 b = 10.42 c = 9.88 β = 88.3°
[0, 1, 0, 0; 1/4, 0, 0, 1; -1/8, 0, 1, 0]
A. Alberti, G. Vezzalini, Acta Crystallogr., B35, 2866 (1979).

GME



GMELINITE



GMELINITE

Framework GME = $[Al_xSi_{24-x}O_{48}]$ x = 8 $P6_3/mmc$ V = 1646 $Å^3$

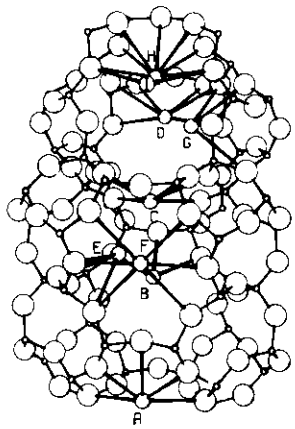
Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	I	$\bar{6}m2[D_{3h}]$	6x2.87
B	II8	$3m[C_{3v}]$	3x2.6
C	III12	$mm[C_{2v}]$	2x3.2 2x3.3
D	IV12	$m[C_s]$	2.7 2x3.1
E	IV12	$m[C_s]$	2.9
F	IV8	$m[C_s]$	3.3 2x3.3

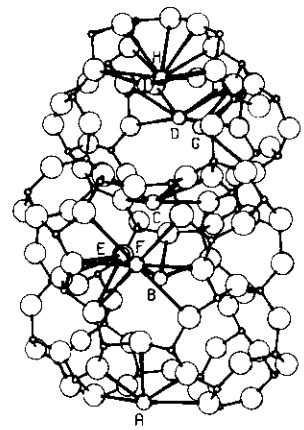
Site occupancies :

site :	A	B	C	D	E	F
(1)	-	4Ca	xH_2O	xH_2O	xH_2O	xH_2O

(1) $(Na_2Ca)_4[8].24H_2O$; h; a = 13.8 c = 10.0
K. Fischer, N. Jahrb. Mineral., Monatsh., 1 (1966).



HEULANDITE



HEULANDITE

Framework HEU = $[Al_xSi_{36-x}O_{72}]$ x = 8 C2/m V = 2104 $\mathring{A}^3$

Extra-framework sites :

site	type	site symmetry	coordination distances ($\mathring{A}$)
A	III8	m[C_s]	2x2.67 3.06 2x3.14
B	IV8	m[C_s]	2.60 2x2.73
C	III8	m[C_s]	2x2.94 2x3.00 2x3.36
D	IV10	m[C_s]	2x3.18 2x3.29 2x3.39
E	IV8	1	3.08 3.35 3.49
F	III8	2/m[C_{2h}]	2x3.05 4x3.40
G	IV10	2[C_2]	3.30 3.34 3.49
H	IV10	m[C_s]	2x3.11 2x3.28 2x3.31 3.39
I	IV10	m[C_s]	2x3.42

Site occupancies :

site :	A	B	C	D	E	F	G	H	I
(1)	0.7Ca 0.8Ca	1Ca	$2H_2O$ $2H_2O$	$0.6H_2O$ $0.4H_2O$	$4H_2O$ $4H_2O$	$2H_2O$	$1.2H_2O$	$2H_2O$ $0.6H_2O$	$0.3H_2O$
(2)	2.8Ca	1.8Ca	$4H_2O$	$3.0H_2O$	$8H_2O$	$2H_2O$	$4H_2O$	$3H_2O$	-
(3)	3Ø	-	1.4Ø	-	-	2Ø	-	2.7Ø	-
(4)a.	1.4M	1.4M	$4H_2O$	$2H_2O$	$7.3H_2O$	$2H_2O$	$3.8H_2O$	$2.7H_2O$	0.4M:::
b.	2.2M	1.8M	$4H_2O$	$2.4H_2O$	$8H_2O$	$2H_2O$	$4.2H_2O$	$2.5H_2O$	0.2M:::
(5)a.	1.6Na 0.8Ca	0.8Na 1.8Ca	1.5K: $3H_2O$	$1.8H_2O$	$8H_2O$	$2H_2O$	0.1Mg::: $3H_2O$	$3.6H_2O$	$1.4H_2O$:::
b.	1.6Na 0.4Ca	0.4Na 1.2Ca	1.8K: $1.5H_2O$	$1.8H_2O$	$8H_2O$	$2H_2O$	0.1Mg::: $3H_2O$	$3.3H_2O$	$1.7H_2O$:::
(6)a.	2M	1.8M	$4H_2O$	$2H_2O$	$7.2H_2O$	$2H_2O$	$2.4H_2O$	$2H_2O$ $1H_2O$	-
b.	2.3M	2.0M	$4H_2O$	$1.4H_2O$	$5.6H_2O$	$1.9H_2O$	$1.6H_2O$	$2.0H_2O$ $1.0H_2O$	-
(7)	-	-	2.4Ca	-	-	0.8Ca:::	-	-	-

(1) $(Ca,Na_2)_4[8].24H_2O$; h; Cm a = 17.73 b = 17.82 c = 7.43 β = 116.3°
[-0.2852, 1, 0, 0; 0, 0, 1, 0; -0.5075, 0, 0, 1]
A.B. Merckle, M. Slaughter, Amer. Mineral., 53, 1120 (1968).
A.B. Merckle, M. Slaughter, Amer. Mineral., 52, 273 (1967).

HEU

*(2) $(Ca,Na_2)_4[8].24H_2O$; h; a = 17.72 b = 17.90 c = 7.43 β = 116.4°
A. Alberti, TMPM Tschermaks Min. Petr. Mitt., 18, 129 (1972).

(3) $(Ca,Na)_4[8].8H_2O$; d; a = 16.95 b = 16.42 c = 7.28 β = 117.8°
A. Alberti, TMPM Tschermaks Min. Petr. Mitt., 19, 173 (1973).

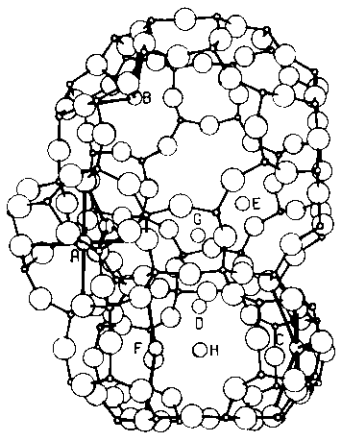
(4) a. $Ca_{1.7}Sr_{0.1}Ba_{0.1}Mg_{0.5}Na_{0.4}K_{1.0}[6.49].23.8H_2O$; h; a = 17.65 b = 17.90 c = 7.40 β = 116.3°
b. $Ca_{1.3}Sr_{0.1}Ba_{0.1}Mg_{0.1}Na_{3.2}K_{1.0}[7.40].21.6H_2O$; h; a = 17.64 b = 18.02 c = 7.40 β = 116.3°
A. Alberti, TMPM Tschermaks Min. Petr. Mitt., 22, 25 (1975).

(5) a. $Ca_{1.9}Na_{1.8}K_{1.0}Mg_{0.2}[6.7].24H_2O$; h; a = 17.66 b = 17.96 c = 7.40 β = 116.5°
b. $Ca_{1.2}Na_{1.8}K_{1.7}Mg_{0.3}[6.3].20H_2O$; h; a = 17.66 b = 17.91 c = 7.41 β = 116.4°
K. Koyama, Y. Takéuchi, Z. Kristallogr., 145, 216 (1977).

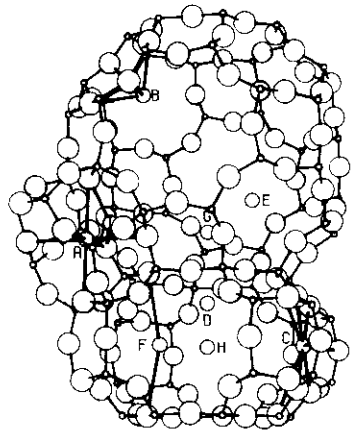
(6) a. $Ca_{3.1}Na_{1.1}K_{0.1}[7.6].24H_2O$; h; a = 17.67 b = 17.93 c = 7.44 β = 116.5°
b. $Ag_{1.3}Ca_{3.1}Na_{0.1}[7.8].25H_2O$; h; a = 17.74 b = 17.97 c = 7.41 β = 116.4°
N. Bresciani-Pahor, M. Calligaris, G. Nardin, L. Randaccio, E. Russo, P. Comin-Chiaramonti, J. Chem. Soc. Dalton Trans., 1511 (1980).

(7) $H_{1.2}K_{0.4}Na_{1.1}Ca_{2.8}[8.3].xH_2O$; d; a = 17.16 b = 17.43 c = 7.39 β = 113.4°
W.J. Mortier, J.R. Pearce, Amer. Mineral., 66, 309 (1981).

KFI



ZK-5



ZK-5

Framework KFI = $[Al_xSi_{96-x}O_{192}]$ x = 30 Im3m V = 6540 $\AA^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	I	$\bar{3}m[D_{3d}]$	6x2.9
B	II8	$3m[C_{3v}]$	3x3.0 3x3.4
C	III8	$\bar{4}2m[D_{2d}]$	4x3.0 4x3.5
D	V8	$4mm[C_{4v}]$	-
E	V8	$mm[C_{2v}]$	-
F	IV8	$mm[C_{2v}]$	2x3.4
G	V8	$4mm[C_{4v}]$	-
H	V8	$4/mmm[D_{4h}]$	-
I	II8	$3m[C_{3v}]$	3x2.3

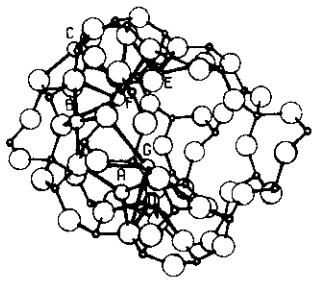
Site occupancies :

site :	A	B	C	D	E	F	G	H	I
(1)a.	-	16Na	-	-	-	-	-	-	-
b.	-	-	-	-	-	-	-	-	-
(2)a.	-	5.4Ba	7.2Ba	4.7Ba	4.3Ba	10.4Cl	2.4Cl, 3.6Cl	-	-
b.	-	3.2Ba	5.8Ba	4.1Ba	-	13.7Br	2.2Br	-	-
c.	-	6.9X, 10.4X	8.9X	11.1X	-	27.8X*	13.0X*	3.8X	-

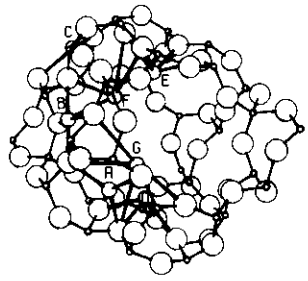
(1) a. $Na_{30}[30].98H_2O$; h; a = 18.75
b. $Na_{30}[30].xH_2O$; d; a = 18.66
W.M. Meier, G.T. Kokotailo, Z. Kristallogr., 121, 211 (1965).

(2) a. $Ba_{15}[30].1.7Ba(OH)_2.12.5BaCl_2.35H_2O$; h; a = 18.65
b. $Ba_{15}[30].1.6Ba(OH)_2.11.9BaBr_2.30H_2O$; h; a = 18.66
c. $(Na,Ba_{0.5})_{30}[30].1.7(Na_2Ba)Cl_2.72H_2O$; h; a = 18.78
R.M. Barrer, D.J. Robinson, Z. Kristallogr., 135, 374 (1972).

LAU



LAUMONTITE



LAUMONTITE

Framework LAU = $[Al_xSi_{24-x}O_{48}]$ x = 8 Am V = 1350 $\mathring{A}^3$

Extra-framework sites :

site	type	site symmetry	coordination distances ($\mathring{A}$)			
A	II10	1	2.33	2.41	2.45	
B	II10	1	2.12	2.16	2.18	2.27
C	II10	1	2.33	2.41	2.45	
D	II10	m[C_s]	2x2.47	2x2.48		
E	II10	m[C_s]	2x2.47	2x2.48		
F	IV10	1	2.85	3.08	3.24	3.29
G	IV10	1	3.21	3.25	3.30	3.41

Site occupancies :

site :	A	B	C	D	E	F	G
(1)	-	-	-	2Ca	2Ca	$4H_2O$	$4H_2O$
(2)	-	-	-	2Ca	2Ca	$2H_2O$, $2H_2O$	$2H_2O$, $2H_2O$
(3)	-	-	-	2Ca	2Ca	$4H_2O$	$4H_2O$
(4)	-	-	-	1.8Ca	1.8Ca	$3.5H_2O$	$4H_2O$

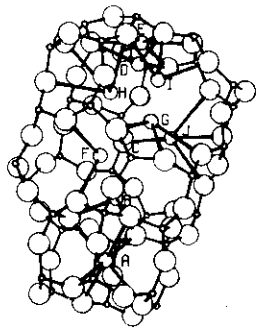
(1) Ca_4[8].$16H_2O$; h; a = 7.57 b = 14.75 c = 13.10 γ = 112°
H. Bartl, K.F. Fischer, Neues Jahrb. Mineral. Mh., 33 (1967).

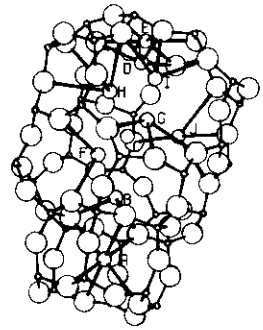
(2) Ca_4[8].xH_2O; h; Cm a = 14.90 b = 13.70 c = 7.55 β = 111.5°
[0, 0, 0, 1; 0, 1, 0, 0; 3/4, 0, 1, 0]
S.T. Amirov, V.V. Ilyukhin, N.V. Belov, Dokl. Akad. Nauk SSSR, 174, 667 (1967).

(3) Ca_4[8].$12H_2O$; h; A2/m a = 7.57 b = 14.82 c = 13.10 γ = 112°
[1/2, 1, 0, 0; 1/2, 0, 1, 0; 0, 0, 0, 1] Protons located
H. Bartl, Neues Jahrb. Mineral. Mh., 298 (1970).

*(4) Ca_4[8].$16H_2O$; h; a = 7.55 b = 14.74 c = 13.07 γ = 111.9°
V. Schramm, K.F. Fischer, Adv. Chem. Ser., 101, 259 (1971).

LEV





Framework LEV = $[Al_xSi_{18-x}O_{36}]$ x = 6.3 $R\bar{3}m$ V = 4089 $Å^3$

Extra-framework sites :

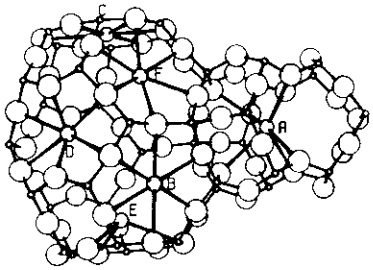
site	type	site symmetry	coordination distances (Å)
A	I	$\bar{3}m[D_{3d}]$	6x2.85
B	II8	$3m[C_{3v}]$	3x2.49
C	V8	$3m[C_{3v}]$	-
D	II8	$3m[C_{3v}]$	3x2.71
E	II8	$\bar{3}m[D_{3d}]$	6x2.59
F	IV8	$m[C_s]$	2.96 3.08
G	IV8	$m[C_s]$	2.98 2.98 3.35
H	IV8	$m[C_s]$	2x3.34 2x3.36
I	IV8	$m[C_s]$	2.54 2x2.74
J	III8	$m[C_s]$	3.02 3.26 3.28 3.31

Site occupancies :

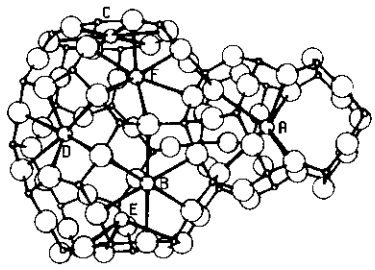
site :	A	B	C	D	E	F	G	H	I	J
(1)	-	6Ca	1.7M	0.9M 1.6M	1.5M	$18H_2O$	$13.1H_2O$	$9.7H_2O$	$4.9H_2O$	-

(1) $Ca_{2.7}Na_{0.7}K_{0.2}[6.3].16.7H_2O$; h; a_{hex} = 13.33 c_{hex} = 23.01
S. Merlino, E. Galli, A. Alberti, TMPM Tschermaks Min. Petr. Mitt., 22, 117 (1975).

LOS



LØSØD



LØSØD

Framework LOS = $[Al_xSi_{24-x}O_{48}]$ x = 12 $P6_3/mmc$ V = 1521 $Å^3$

Extra-framework sites :

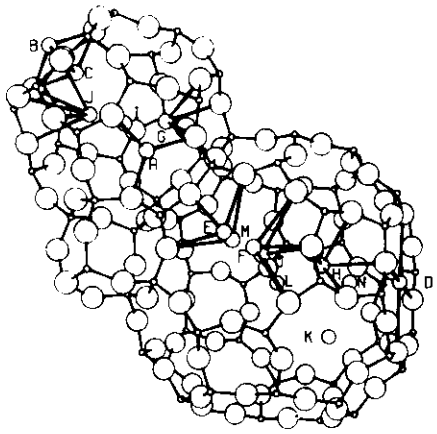
site	type	site symmetry	coordination distances (Å)	
A	II6	$\bar{6}m2[D_{3h}]$	6x3.25	
B	II6	$2/m[C_{2h}]$	6x2.70	
C	II6	$\bar{6}m2[D_{3d}]$	6x2.90	
D	II6	$mm[C_{2v}]$	2x2.4	4x2.9
E	II6	$3m[C_{3v}]$	3x3.4	
F	II6	$m[C_s]$	2x2.8	4x2.8

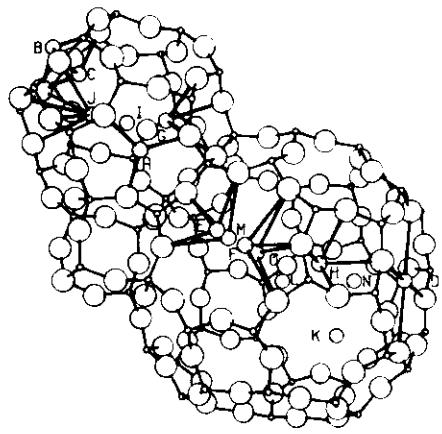
Site occupancies :

(1) no cations or water molecules located.

(1) $Na_{12}[12].18H_2O$; h; a = 12.91 c = 10.54
W. Sieber, W.M. Meier, Helv. Chim. Acta, 57, 1533 (1974).

LTA





Framework LTA = $[Al_xSi_{24-x}O_{48}]$ x = 12 Pm3m V = 1860 $\mathring{A}^3$

Extra-framework sites :

site	type	site symmetry	coordination distances ($\mathring{A}$)		
A	II8	$3m[C_{3v}]$	3x2.30		
B	II8	$3m[C_{3v}]$	3x2.50		
C	II6	$3m[C_{3v}]$	3x2.50		
D	III8	$4/mmm[D_{4h}]$	4x3.40		
E	III8	$mm[C_{2v}]$	2.50	2x2.80	
F	III8	$mm[C_{2v}]$	2.70	2x3.10	3.50
G	IV6	$4mm[C_{4v}]$	3x2.85		
H	IV8	$mm[C_{2v}]$	4x3.10		
I	V6	$m3m[O_h]$	-		
J	IV6	$mm[C_{2v}]$	4x3.25	3.40	
K	V8	$3m[C_{3v}]$	-		
L	V8	$m3m[O_h]$	-		
M	III8	$m[C_s]$	2.80	2x3.00	
N	V8	$4mm[C_{4v}]$	-		
O	V8	$m[C_s]$	2.94	2x3.34	

Site occupancies :

site :	A	B	C	D	E	F	G	H
(1)a.	8Na	-	-	-	4Na	-	-	-
b.	-	8Tl	-	-	4Na	-	-	-
c.	8Li	-	-	-	4Na	-	-	-
(2)	-	8Na*	-	-	-	-	-	-
	+ other sites : 4Na(O)							
(3)a.	8Na	-	-	-	-	-	-	-
b.	8Na, Ca	-	-	-	-	-	-	-
(4)	-	8Na	-	-	-	-	-	11Br***
	+ other sites : 1Na(I)							
(5)a.	4Ca	-	4Na	-	-	-	-	-
b.	4Ca, 4Na	-	-	-	-	-	-	5.5I***
	+ other sites : 5.5I***(N)							

LTA

Site occupancies :

site :	A	B	C	D	E	F	G	H
(6)	-	8Na	-	-	-	-	-	-
	+ other sites : 4Na(O)							
(7)	-	64Na	-	-	-	-	-	$125H_2O^{xxx}$
	+ other sites : $44H_2O^{xxx}$(I); $58H_2O$(K); $15H_2O$(L); $84H_2O$ (O)^{x}							
(8)a.	-	7Tl	1Tl	-	3Tl	-	-	-
b.	-	7Tl	1Tl	-	3Tl	-	-	-
(9)	-	8Na	8N	-	-	-	4N	$12N^{x}$
	+ other sites : 8N(K); 3Na(M)							
(10)	8Na	-	-	-	3Na	-	-	$8S^{x}$
	+ other sites : $8S^{x}$(K)							
(11)	8Na	-	-	-	3Na	-	-	1Na
	+ other sites : $6C^{x}$(K); $3C^{x}$(N); 3C(O)							
(12)a.	3Co	4Na	-	-	-	-	-	-
b.	-	3Co, 4Na	-	-	-	-	-	-
	+ other sites : 1Co(I)							
(13)	8Na	-	-	-	3Na	-	-	1Na
(14)	8Na	-	-	-	3Na	-	-	1Na
(15)a.	4.5Mn, 3Na	-	-	-	-	-	-	-
b.	4.5Mn	-	xH_2O	-	-	-	-	-
	+ other sites : xH_2O(K)							
(16)	-	4.5Mn	3Na	-	-	-	-	-
	+ other sites : $9C^{x}$(K)							
(17)a.	4.5Mn	-	$4.5H_2O$	-	-	-	-	$12H_2O^{x}$
	+ other sites : 1(Na,H_2O)(I); $6H_2O$(K); 3(Na,H_2O)(N); 3(Na,H_2O)(O)							
b.	4.5Mn, 3Na	-	-	-	-	-	-	-
(18)a.	4Co	-	4Na	-	-	-	-	-
b.	-	4Co	4Na	-	-	-	-	-
	+ other sites : 4C, $4\emptyset^{xxx}$(K)							
(19)	-	4Co	4Na	-	-	-	-	-
	+ other sites : $8C^{x}$(K)							
(20)a.	4.5Mn	-	3Na	-	-	-	-	-
	+ other sites : $9C^{x}$(K)							
b.	4Na	4Co	-	-	-	-	-	-
	+ other sites : $8C^{x}$(K)							
(21)	1Na	3Co	2Na	-	-	-	-	$9H_2O^{x}$
	+ other sites : 1Co(I); $6H_2O^{x}$(J); $3H_2O^{xxx}$(K); $2H_2O$, $3H_2O^{xxx}$, $3H_2O^{xxx}$(M); 1Na(N)							
(22)a.	1K	6K	1K, 1K	-	3K	-	-	-
b.	-	8K	$8H_2O$	-	-	-	-	$12H_2O$
	+ other sites : $1K^{xxx}$(L); 3K(M)							
(23)a.	4Na	-	1Cs	3Cs	-	-	-	-
	+ other sites : 3Cs(K)							
b.	-	4Na	1Cs	3Cs	-	-	-	-
	+ other sites : 3Cs(K)							
(24)	6.7Na	-	-	-	-	-	-	10Na
	+ other sites : 6.7Ø(J); 7.2N, $19.4\emptyset^{xxx}$, 4.2Ø(K); 1Na, $2.2\emptyset^{xxx}$(L), $11H_2O$(M); 4.4Na(N)							
(25)a.	-	5.8Tl	1.6Tl	-	$2.4Tl^{x}$	-	-	$8.4H_2O^{xxx}$
	+ other sites : $3.8H_2O$(J)							
b.	3Ca	3Ca	$2.8H_2O$	$1H_2O$	-	-	-	-
	+ other sites : $0.4H_2O$(I); $4.2H_2O$(K); $2.4H_2O^{xxx}$(L); $10.6H_2O$(M)							

Site occupancies : continued.

site :	A	B	C	D	E	F	G	H
(25)c.	-	4.9Ag	2.6Ag	-	-	-	$3.6H_2O$	-
	+ other sites : $12H_2O$(O)							
(26)	1Na	5Rb	2Rb	3Rb	-	-	-	-
	+ other sites : 1Rb(K)							
(27)	1.5Zn	2.5Zn	1Zn	-	-	1K	-	-
	+ other sites : $1H_2O^{\ddagger\ddagger}$(I); $2.5H_2O$(K); 1K(M)							
(28)a.	1Na	5Rb	1Rb, 1Rb	3Rb	-	-	-	-
	+ other sites : 1Rb(K)							
b.	-	5Rb	2Rb	1Rb	-	-	-	$1Rb^{\ddagger\ddagger}$, $4H_2O$
	+ other sites : $3H_2O$(J); 2Rb(M)							
(29)a.	-	6Tl	2Tl	-	3Tl	-	-	-
	+ other sites : 1Tl(K)							
b.	-	7Tl	1Tl	-	3Tl	-	-	$3H_2O$, $6H_2O^{\ddagger\ddagger}$
	+ other sites : $1Tl^{\ddagger}$(J)							
(30)	3K	3Cs	1Cs, 1K	3Cs	-	-	-	-
	+ other sites : 1K(K)							
(31)a.	8Ag	-	-	-	2Ag	-	2Ag	-
b.	8Ag	-	-	-	$0.5Ag^{\ddagger}$	-	3.5Ag	-
(32)	-	4Ag	2Ag	-	2Ag	-	1N	$4N^{\ddagger}$
	+ other sites : 3N(J); $12N^{\ddagger}$(K)							
(33)	3Eu	-	1Eu	1Eu	-	-	-	0.8Eu
(34)	8Na	-	-	-	3Na	-	-	1Na
(35)	2.6Ag	3.8Ag	0.6Ag	-	0.7Ag	-	2.6Ag	-
	+ other sites : $7.5C^{\ddagger\ddagger}$(K); 1.0Ag(O)							
(36)	2.6Eu	-	1.2Eu	-	1.6Na	-	-	0.5Eu, 2.4Ø
(37)	4.3Eu	-	4Cl	-	-	-	-	-
	+ other sites : 4Cl(K); 1Eu(N)							
(38)	8Ag	-	-	-	3Ag	-	0.6Ag	-
(39)	4.4Ag	3.6Ag	-	-	1.8Ag	-	-	$3.6Br^{\ddagger}$
	+ other sites : $3.6Br^{\ddagger\ddagger}$(K); $2.4Br^{\ddagger\ddagger}$(N); 2.4Br(O)							
(40)a.	3Ag, 2Ag	-	3Ag	-	-	1Ag	3Ø	1Ag
	+ other sites : $2Ag^{\ddagger}$(M)							
b.	-	5Ag	3Ag	-	-	-	-	$1Ag^{\ddagger}$
	+ other sites : $3H_2O^{\ddagger\ddagger}$(I); 1Ag(M); $1Ag^{\ddagger\ddagger}$(N); 1Ag(O)							
(41)	4Ag	2.5Tl	1.5Ag	-	1.5Tl	-	1Ag	-
	+ other sites : 1.5Tl(O)							
(42)a.	1Ca	3Ca	1Ca	-	1Ca	-	-	-
b.	3Sr	-	2Sr	-	-	-	-	-
	+ other sites : 1Sr(M)							
(43)a.	4Na	3Ni	$4H_2O^{\ddagger}$	-	-	-	-	$9H_2O^{\ddagger}$
	+ other sites : $4H_2O$(K); $4H_2O$(O)							
b.	4Na	4Fe	$4.8H_2O^{\ddagger}$	-	-	-	-	$6H_2O^{\ddagger}$
	+ other sites : 0.7Fe(I); $4H_2O$(O)							
(44)	-	3.3Eu	0.5Eu, $7.4H_2O^{\ddagger}$	-	-	-	-	$10.6H_2O^{\ddagger}$
	+ other sites : $3H_2O^{\ddagger\ddagger}$(K); 1Eu(M)							
(45)a.	-	4.0Cd	3.0Cd	0.5Cd	-	-	-	$2Cd^{\ddagger}$
	+ other sites : $4Cl^{\ddagger}$(K); 3ØH(M)							

LTA

Site occupancies : continued.

site :	A	B	C	D	E	F	G	H
(45)b.	3Cd	2Cd	1Cd, 3ØH	1Cd	-	-	-	3Ø$^{:::}$
	+ other sites : 1Cd(K); 1Ø$^{:::}$(L); 2Cl$^{:::}$, 1.5Cd$^{:::}$(M); 2Cl(N)							
(46)	-	4Co	-	-	-	1Na	-	4Cl$^{:::}$
	+ other sites : 4Cl(K); 2Na(O)							
(47)	5.2Ag	2.2Ag	-	-	-	-	-	2.4Ag, 2.9Ag^{x}
	+ other sites : 2.2Ag(K); 6Cl, 6.2Cl(O)							
(48)a.	5.2Ag	-	-	-	0.4Ag	-	1.9Ag	-
b.	8Ag	-	-	-	0.6Ag	1.4Ag	0.3Ag	0.3Ag
c.	7.3Ag	-	-	-	2Ag	-	2Ag	-
d.	8Ag	-	-	-	0.2Ag^{x}	-	3.5Ag	-
e.	7.8Ag	-	-	-	-	-	3.5Ag	-
f.	6.8Ag	-	-	-	-	-	2.5Ag	-
(49)a.	4Na	6Co	-	-	-	-	-	-
	+ other sites : 12C^{x}(K)							
b.	4Mn	-	4Na	-	-	-	-	-
	+ other sites : 12C^{x}(K)							
(50)a.	-	6.3K	1.4K	-	3K	-	0.1K	0.3K
b.	-	49.6K	12.3K	-	24K	-	1.2K	4K
(51)a.	4Co	-	1Na	-	3Na	-	-	-
	+ other sites : 3N, 3Ø$^{:::}$(K)							
b.	4Na	6Co	-	-	-	-	-	-
	+ other sites : 2N, 2Ø$^{:::}$, 2Ø$^{:::}$(K)							
(52)	-	4Cs	2Tl	2Cs^{x}, 1Cs	-	-	-	1Tl^{x}
	+ other sites : 2Cs(K)							
(53)a.	3Cd	1Cd	2Cd, 1Cd	-	-	-	-	-
	+ other sites : 1Cd$^{:::}$(I); 3Ø(K); 1Cd(M)							
b.	3Cd	-	3Cd	-	-	-	-	-
	+ other sites : 3Ø$^{:::}$(I)							
(54)	1Co	3Co	2Na	-	2Na	-	-	3C
	+ other sites : 3S(K)							
(55)	62.2Na	-	-	23.2Na	-	-	-	6.3Na
(56)	-	3Zn, 5Ø	-	1Ø^{x}	2Na	-	-	3Ø, 4Ø^{x}, 4Ø^{x}
	+ other sites : 1Zn(I); 1Zn(N); 6Ø^{x}(J); 1Ø$^{:::}$(N)							
(57)a.	3.6Cd	-	2.2Cd	-	-	-	-	-
	+ other sites : 1.7Ø$^{:::}$(I)							
b.	3.2Cd	-	2.6Cd	-	-	-	-	-
	+ other sites : 2.3Ø$^{:::}$(I)							
(58)a.	5Ca	-	-	1.7Cs	-	-	-	-
b.	3.3Ca	0.8Cs, 0.7Ca	0.4Cs	3Cs	-	-	-	-
c.	2.3Ca	1.4Cs	0.7Cs, 1.0Ca	3.0Cs	-	-	-	-
d.	3.0Ca	2.1Cs	1.2Cs	3.0Cs	-	-	-	-
e.	2.8Ca	2.3Cs	1.0Cs	3.0Cs	-	-	-	-
(59)a.	3.0Cd	1.4Cd	1.5Cd, 3.8Ø	-	-	-	-	10.0Ø^{x}
	+ other sites : 5.8Ø(K); 7.0Ø$^{:::}$(K); 5.6Ø(O); 2.3Ø(K)							
b.	3.0Cd	1.5Cd	1.5Cd, 1.7Ø^{x}	-	1.5Ø	-	-	-
	+ other sites : 2.0Ø(J); 0.8Ø(K)							
(60)	2.0Ag, 1.9Ag	2.1Na	-	-	2Na, 1Ag	-	1.0Ag	-

Site occupancies : continued.

site :	A	B	C	D	E	F	G	H
(61)a.	4.8Cu	0.9Cu	-	-	-	-	-	2.0Cu
	+ other sites : 1.0ØH$^{\cdots}$(I); 1.0ØH(K); 1.0ØH(K)							
b.	4.9Cu	-	-	-	2.0Cu	-	-	1.3Cu
	+ other sites : 2.3ØH$^{\cdots}$(I)							
c.	4.8Cu	0.8Cu	-	-	-	-	0.5Cu	1.4Cu
	+ other sites : 0.2Cu(I); 1.4Cu$^{\cdots}$(I)							
d.	5.7Cu	-	-	-	-	-	-	-
(62)a.	-	4Zn	-	1.0Ø	-	-	-	1Zn, 8.0Ø$^{\cdots}$
	+ other sites : 1Zn(I); 4Ø$^{\cdots}$(I); 8Ø(K); 4.0Ø(O); 2.0Ø(N); 2.0Ø$^{\cdots}$(L)							
b.	4.0Zn	-	2.0Zn	-	-	-	-	-
	+ other sites : 2.0Ø$^{\cdots}$(I)							

(1) a. Na_{12}[12]; d; a = 12.32
b. $Tl_{9.6}Na_{2.4}$[12]; d; a = 12.33
c. Li_8Na_4[12]; d; a = 12.04
T.B. Reed, D.W. Breck, J. Am. Chem. Soc., 78, 5972 (1956).

(2) Na_{12}[12]; d; a = 12.28
P.A. Howell, Acta Crystallogr., 13, 737 (1956).

(3) a. Na_{12}[12].xH_2O; h; a = 12.30
b. Na_4Ca_4[12].xH_2O; h; a = 12.30
L. Broussard, D.P. Shoemaker, J. Am. Chem. Soc., 82, 1041 (1960).

(4) Na_{12}[12].xBr_2; d+Br_2; a = 12.30
W.M. Meier, D.P. Shoemaker, Z. Kristallogr., 123, 5 (1966)

(5) a. Ca_4Na_4[12]; d; a = 12.42
b. Ca_4Na_4[12].5.65I_2; d+I_2; a = 12.29
K. Seff, D.P. Shoemaker, Acta Crystallogr., 22, 162 (1967).

(6) Na_{12}[12]; d; a = 12.28
J.V. Smith, L.G. Dowell, Z. Kristallogr., 126, 1 (1968).

(7) Na_{96}[8x12].216H_2O; h; $Fm\bar{3}c$ a = 24.61
[0, 2, 0, 0; 0, 0, 2, 0; 0, 0, 0, 2]
V. Gramlich, W.M. Meier, Z. Kristallogr., 133, 134 (1971).

(8) a. Tl_{12}[12]; d; a = 12.17
b. Tl_{12}[12].xH_2O; h; a = 12.32
P.E. Riley, K. Seff, D.P. Shoemaker, J. Phys. Chem., 76, 2593 (1972).

(9) Na_{11}[11].32NH_3; d+NH_3; a = 12.29
R.Y. Yanagida, K. Seff, J. Phys. Chem., 76, 2597 (1972).

(10) Na_{11}[11].16S; d+S; a = 12.29
K. Seff, J. Phys. Chem., 76, 2601 (1972).

(11) Na_{12}[12].6C_2H_2; d+C_2H_2; a = 12.26
A.A. Amaro, K. Seff, J. Phys. Chem., 77, 906 (1973).

(12) a. Na_4Co_4[12]; d;
b. Na_4Co_4[12].xH_2O; h;
P.E. Riley, K. Seff, J. Chem. Soc., Chemical Comm., 1287 (1972).

(13) Na_{12}[12].xNH_3; d+NH_3; a = 12.29
R.Y. Yanagida, K. Seff, J. Phys. Chem., 77, 138 (1973).

(14) Na_{12}[12]; d; a = 12.26
R.Y. Yanagida, A.A. Amaro, K. Seff, J. Phys. Chem., 77, 805 (1973).

LTA

(15) a. $Mn_{4.5}Na_3[12]$; d; a = 12.18
b. $Mn_{4.5}Na_3[12].xH_2O$; h; a = 12.27
R.Y. Yanagida, T.B. Vance, K. Seff, J. Chem. Soc., Chem. Comm., 382 (1973).

(16) $Mn_{4.5}Na_3[12].4.5C_2H_2$; d+$C_2H_2$; a = 12.21
P.E. Riley, K. Seff, J. Am. Chem. Soc., 95, 8180 (1973).

(17) a. $Mn_{4.5}Na_3[12].xH_2O$; h; a = 12.27
b. $Mn_{4.5}Na_3[12]$; d; a = 12.18
R.Y. Yanagida, T.B. Vance, K. Seff, Inorg. Chem., 13, 723 (1974).

(18) a. $Co_4Na_4[12]$; d; a = 12.09
b. $Co_4Na_4[12].4CO$; d+CO; a = 12.09
P.E. Riley, K. Seff, Inorg. Chem., 13, 1355 (1974).

(19) $Co_4Na_4[12].4C_2H_4$; d+C_2H_4; a = 12.14
P.E. Riley, K.B. Kunz, K. Seff, J. Am. Chem. Soc., 97, 537 (1975).

(20) a. $Mn_{4.5}Na_3[12].4.5C_2H_2$; d+$C_2H_2$; a = 12.21
b. $Co_4Na_4[12].4C_2H_2$; d+C_2H_2; a = 12.17
P.E. Riley, K. Seff, Inorg. Chem., 14, 714 (1975).

(21) $Co_4Na_4[12].xH_2O$; h; a = 12.27 Å
[+ oxygen position at 1.74 Å from T]
P.E. Riley, K. Seff, J. Phys. Chem., 79, 1594 (1975).

(22) a. $K_{12}[12]$; d; a = 12.31
b. $K_{12}[12].xH_2O$; h; a = 12.30
P.C.W. Leung, K.B. Kunz, K. Seff, I.E. Maxwell, J. Phys. Chem., 79, 2157 (1975).

(23) a. $Cs_7Na_5[12]$; d; a = 12.16
b. $Cs_7Na_5[12].xH_2O$; h; a = 12.32
T.B. Vance, K. Seff, J. Phys. Chem., 79, 2163 (1975).

(24) $Na_{12}[12].9.3NaNO_3.6.7H_2O$; h+$NaNO_3$; a = 12.39
R.M. Barrer, H. Villiger, Z. Kristallogr., 142, 82 (1975).

(25) a. $Tl_{12}[12].18H_2O$; h; a = 12.35
b. $Ca_6[12].28H_2O$; h; a = 12.24
c. $Ag_{12}[12].23H_2O$; h; a = 12.30
W. Thöni, Z. Kristallogr., 142, 142 (1975).

(26) $Rb_{11}Na_1[12]$; d; a = 12.26
R.L. Firor, K. Seff, J. Am. Chem. Soc., 98, 5031 (1976).

(27) $Zn_5K_2[12]$; d; a = 12.08
N.V. Raghavan, K. Seff, J. Phys. Chem., 80, 2133 (1976).

(28) a. $Rb_{11}Na_1[12]$; d; a = 12.26
b. $Rb_{11}Na_1[12].xH_2O$; h; a = 12.32
R.L. Firor, K. Seff, J. Am. Chem. Soc., 99, 1112 (1977).

(29) a. $Tl_{12}[12]$; d; a = 12.18
b. $Tl_{12}[12].xH_2O$; h; a = 12.38
R.L. Firor, K. Seff, J. Am. Chem. Soc., 99, 4039 (1977).

(30) $Cs_7K_5[12]$; d; a = 12.27
R.L. Firor, K. Seff, J. Am. Chem. Soc., 99, 6249 (1977).

(31) a. $Ag_{12}[12]$; d; a = 12.30
b. $Ag_{12}[12]$; d; a = 12.30
Y. Kim, K. Seff, J. Am. Chem. Soc., 99, 7055 (1977).

(32) $Ag_{12}[12].xNH_3$; d+NH_3; a = 12.30
[+ 2N located near the center of the small cubic cavity]
Y. Kim, J.W. Gilje, K. Seff, J. Am. Chem. Soc., 99, 7057 (1977).

(33) Eu_6[12]; d; a = 12.30
R.L. Firor, K. Seff, J. Am. Chem. Soc., 99, 7059 (1977).

(34) Na_{12}[12]; d; a = 12.29
V. Subramanian, K. Seff, J. Phys. Chem., 81, 2249 (1977).

(35) Ag_{12}[12].xC_2H_4; d+C_2H_4; a = 12.21
Y. Kim, K. Seff, J. Am. Chem. Soc., 100, 175 (1978).

(36) $Eu_{4.5}Na_3$[12]; d+O_2; a = 12.24
R.L. Firor, K. Seff, J. Am. Chem. Soc., 100, 976 (1978).

(37) $Eu_{5.5}$Na[12].xCl_2; d+Cl_2; a = 12.25
R.L. Firor, K. Seff, J. Am. Chem. Soc., 100, 978 (1978).

(38) Ag_{12}[12]; d+H_2+O_2; a = 12.30
Y. Kim, K. Seff, J. Phys. Chem., 82, 921 (1978).

(39) Ag_{12}[12].6Br_2; d+Br_2; a = 12.26
Y. Kim, K. Seff, J. Phys. Chem., 82, 925 (1978).

(40) a. Ag_{12}[12]; d; a = 12.29
b. Ag_{12}[12].xH_2O; h; a = 12.21
Y. Kim, K. Seff, J. Phys. Chem., 82, 1071 (1978).

(41) $Ag_{6.5}Tl_{5.5}$[12]; d; a = 12.25
Y. Kim, K. Seff, J. Phys. Chem., 82, 1307 (1978).

(42) a. Ca_6[12]; d; a = 12.28
b. Sr_6[12]; d; a = 12.32
R.L. Firor, K. Seff, J. Am. Chem. Soc., 100, 3091 (1978).

(43) a. Ni_3Na_6[12].xH_2O; h; a = 12.26
[+ oxygen at 1.2 Å from T]
b. $Fe_{2.7}Na_{6.6}$[12].xH_2O; h; a = 12.24
R.L. Firor, K. Seff, J. Phys. Chem., 82, 1650 (1978).

(44) Eu_5Na_2[12].xH_2O; h; a = 12.29
R.L. Firor, K. Seff, Inorg. Chem., 17, 2144 (1978).

(45) a. $Cd_{9.5}Cl_4(OH)_3$[12]; d; a = 12.27
b. $Cd_{9.5}Cl_4(OH)_3$[12].xH_2O; d; a = 12.22
L.B. McCusker, K. Seff, J. Am. Chem. Soc., 100, 5052 (1978).

(46) Co_4Na_4[12].4Cl_2; d+Cl_2; a = 12.10
V. Subramanian, K. Seff, T. Ottersen, J. Am. Chem. Soc., 100, 2911 (1978).

(47) $H_{2.3}Ag_{12}Cl_{2.3}$[12].6Cl_2; d+Cl_2; a = 12.24
Y. Kim, K. Seff, J. Am. Chem. Soc., 100, 3801 (1978).

(48) a. Ag_{12}[12]; d; a = 12.28
b. Ag_{12}[12]; d; a = 12.33
c. Ag_{12}[12]; d; a = 12.30
d. Ag_{12}[12]; d; a = 12.30
e. Ag_{12}[12]; d; a = 12.25
f. Ag_{12}[12]; d; a = 12.15
Y. Kim, K. Seff, J. Am. Chem. Soc., 100, 6989 (1978).

(49) a. Co_4Na_4[12].4C_3H_6; d+C_3H_6; a = 12.15
b. Mn_4Na_4[12].4C_3H_6; d+C_3H_6; a = 12.15
W.V. Cruz, P.C.W. Leung, K. Seff, J. Am. Chem. Soc., 100, 6997 (1978).

(50) a. K_{12}[12]; d; a = 12.32
b. K_{96}[8x12]; d; $Fm\bar{3}c$ a = 24.60
[0, 2, 0, 0; 0, 0, 2, 0; 0, 0, 0, 2]
J.J. Pluth, J.V. Smith, J. Phys. Chem., 83, 741 (1979).

LTA

(51) a. Co_4Na_4[12].3NO; d+NO; a = 12.19

b. Co_4Na_4[12].2NO_2; d+NO_2; a = 12.14

W.C. Cruz, P.W. Leung, K. Seff, Inorg. Chem., 18, 1692 (1979).

(52) Cs_9Tl_3[12]; d; a = 12.31

V. Subramanian, K. Seff, J. Phys. Chem., 83, 2166 (1979).

(53) a. $[Cd(H_2O)]_3Cd_3$[12]; d; a = 12.24

b. $[Cd^{II}_2(H_2O)]_3Cd^{I}_3[Cd^{I}_2]_{1.5}$[12]; d; a = 12.29

L.B. McCusker, K. Seff, J. Am. Chem. Soc., 101, 5235 (1979).

(54) $(CoSCH_3)_3CoNa_4$[12]; d+$(CH_3)_2S$; a = 12.20

V. Subramanian, K. Seff, J. Am. Chem. Soc., 102, 1881 (1980).

(55) Na_{96}[8x12]; d; $Fm\bar{3}c$ a = 24.56

[0, 2, 0, 0; 0, 0, 2, 0; 0, 0, 0, 2]

J.J. Pluth, J.V. Smith, J. Am. Chem. Soc., 102, 4704 (1980).

(56) Zn_5Na_2[12].xH_2O; h; a = 12.20

Y. Kim, K. Seff, J. Phys. Chem., 84, 2823 (1980).

(57) a. Cd_6[12]; d; a = 12.26

b. Cd_6[12]; d; a = 12.24

L.B. McCusker, K. Seff, J. Phys. Chem., 84, 2827 (1980).

(58) a. $Ca_{5.1}Cs_{1.7}$[12]; d; a = 12.28

b. $Ca_{4.0}Cs_{4.0}$[12]; d; a = 12.20

c. $Ca_{3.4}Cs_{5.3}$[12]; d; a = 12.23

d. Ca_3Cs_6[12]; d; a = 12.23

e. $Ca_{2.8}Cs_{6.4}$[12]; d; a = 12.24

V. Subramanian, K. Seff, J. Phys. Chem., 84, 2928 (1980).

(59) a. Cd_6[12].xH_2O; h; a = 12.23

b. Cd_6[12].xH_2O; d; a = 12.24

L.B. McCusker, K. Seff, J. Phys. Chem., 85, 166 (1981).

(60) $Na_{5.5}Ag_{6.5}$[12]; d; a = 12.32

L.R. Gellens, W.J. Mortier, J.B. Uytterhoeven, Zeolites, 1, 11 (1981).

(61) a. $Cu^{II}_5Cu^{I}_3$[12].ØH.xH_2O; d; a = 12.15

b. Cu^{II}_8[12].4ØH.xH_2O; d+O_2+d; a = 12.18

c. $Cu^{II}_5Cu^{I}_{2.5}Cu^{\circ}_{0.5}$[12].0.5ØH.x$H_2O$; d; a = 12.19

d. Cu^{II}_6[12]; d; a = 12.21

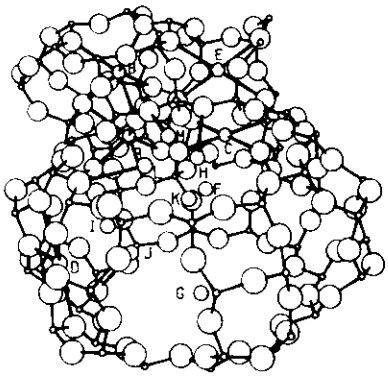
H.S. Lee, K. Seff, J. Phys. Chem., 85, 397 (1981).

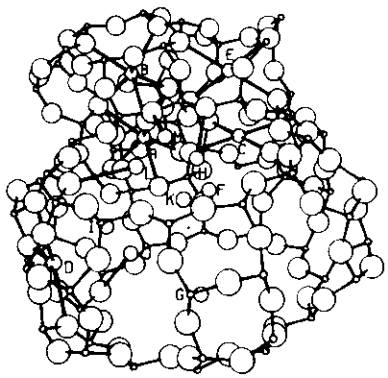
(62) a. Zn_6[12].xH_2O; h; a = 12.16

b. Zn_6[12]; d; a = 12.05

L.B. McCusker, K. Seff, J. Phys. Chem., 85, 405 (1981).

LTL





Framework LTL = $[Al_xSi_{36-x}O_{72}]$ x = 9 P6/mmm V = 2205 $Å^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	I	$\bar{6}m2[D_{3h}]$	6x3.00
B	II6	$\bar{6}m2[D_{3h}]$	6x2.90
C	IV8	$mmm[D_{2h}]$	4x2.83
D	III12	$mm[C_{2v}]$	2x2.36 4x2.96
E	IV8	$mmm[D_{2h}]$	4x2.90
F	V12	$mm[C_{2v}]$	-
G	V12	$6/mmm[D_{6h}]$	-
H	IV12	$m[C_s]$	2.79
I	V12	$m[C_s]$	-
J	IV12	$m[C_s]$	3.05
K	V12	$6mm[C_{6v}]$	-
L	IV12	$mm[C_{2v}]$	3.08
M	IV12	$mm[C_{2v}]$	3.01

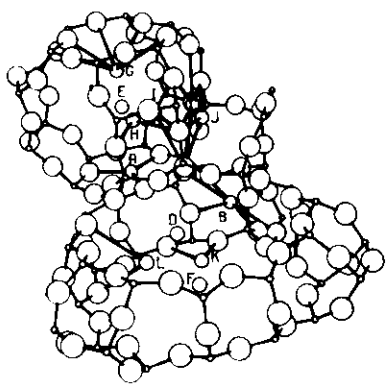
Site occupancies :

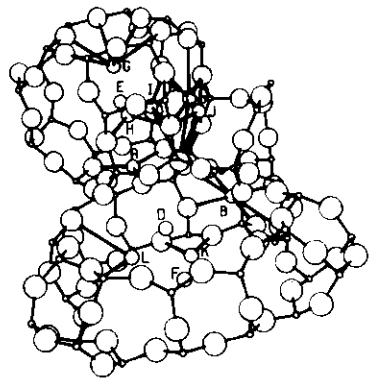
site :	A	B	C	D	E	F	G	H	I	J	K	L	M
(1)	1.4Na, K	2K	-	3.6Na	1.8K	$3H_2O$	$0.5H_2O$	$3H_2O$	$4.2H_2O$	$3H_2O$	$1.4H_2O$	$1.5H_2O$	$4.2H_2O$
(2)	-	2Ba	-	4.4K, Ba	2.5Ba	5.1Ø	-	12Ø	5.7Ø	4.8Ø	-	-	-

(1) $Na_3K_6[9].21H_2O$; h; a = 18.40 c = 7.52
R.M. Barrer, H. Villiger, Z. Kristallogr., 128, 352 (1969).

(2) $K_{2.7}Ba_{7.7}[18].23H_2O$; h; a = 18.70 c = 7.50
Ch. Baerlocher, R.M. Barrer, Z. Kristallogr., 136, 245 (1972).

MAZ





Framework MAZ = $[Al_xSi_{36-x}O_{72}]$ x = 10 $P6_3/mmc$ V = 2243 $Å^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	II6	$\bar{6}m2[D_{3h}]$	3x2.37
B	III6	$2/m[C_{2h}]$	4x2.89 2x3.07
C	III6	$m[C_s]$	3.03 3.16 2x3.29 2x3.37
D	V12	$mm[C_{2v}]$	-
E	V6	$\bar{6}m2[D_{3h}]$	-
F	V12	$3m[C_{3v}]$	-
G	II6	$3m[C_{3v}]$	3x2.97 3x3.42
H	IV6	$mm[C_{2v}]$	2x3.04
I	IV6	$m[C_s]$	2.97 2x3.30
J	III6	$m[C_s]$	2x2.92 2x3.22 3.40
K	IV12	1	2.62 3.00
L	IV12	1	3.20 3.39

Site occupancies :

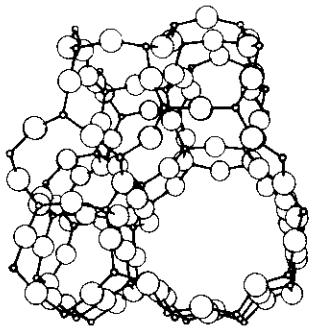
site :	A	B	C	D	E	F	G	H	I	J
(1)	-	2.8M	-	$4.9H_2O$	2Mg	0.8Ca	$4H_2O$	$2.4H_2O$	$3.6H_2O$	$6.8H_2O$
(2)	1.9Mg*	1.7Ca	$6.6H_2O$	1.5K	$2.3H_2O$*	-	-	-	-	-

	K	L
(1)	$6H_2O$	$4.7H_2O$
(2)	-	-

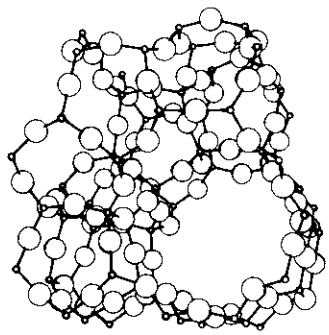
(1) $K_{1.9}Mg_{2.0}Ca_{1.4}[9.77].28H_2O$; h; a = 18.40 c = 7.65
E. Galli, Cryst. Struct. Comm., 3, 339 (1974).

(2) $Na_{0.3}K_{2.5}Ca_{1.4}Mg_{2.1}[9.9].xH_2O$; d; a = 18.01 b = 7.61
R. Rinaldi, J.J. Pluth, J.V. Smith, Acta Crystallogr., B31, 1603 (1975).

MEL



ZSM-11



ZSM-11

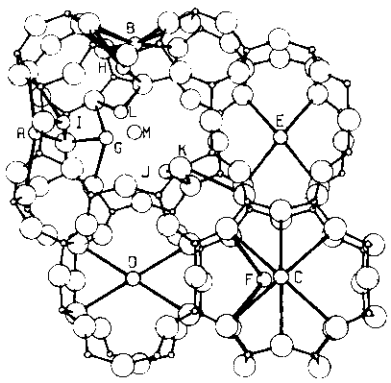
Framework MEL = $[Al_xSi_{96-x}O_{192}]$ $x < 16$ $I\bar{4}m2$ $V = 5440$ Å^3

No extra-framework sites detected.

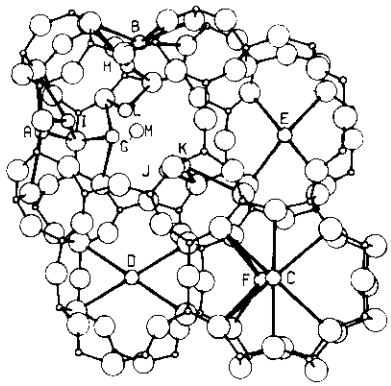
Reference :

(1) Simulated model of ZSM-11, a = b = 20.12 c = 13.44
G.T. Kokotailo, P. Chu, S.L. Lawton, W.M. Meier, Nature, 275, 119 (1978).

MER



MERLINOITE



MERLINOITE

Framework MER = $[Al_xSi_{32-x}O_{64}]$ x = 9 Immm V = 2000 $\AA^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	III8	mm[C_{2v}]	2x3.1 2x3.1
B	III8	mm[C_{2v}]	2x2.9 2x3.1 2x3.4
C	III8	mm[C_{2v}]	2x3.1 4x3.4
D	IV8	mmm[D_{2h}]	4x3.2
E	III8	mm[C_{2v}]	4x3.1
F	IV8	mm[C_{2v}]	4x3.4
G	IV8	m[C_s]	2.6 2x2.8
H	IV8	m[C_s]	3.1 2x3.2 2x3.2
I	IV8	m[C_s]	2x3.0 3.1
J	IV8	m[C_s]	2x3.2
K	IV8	m[C_s]	2x3.2 3.3
L	IV8	1	3.2 3.3
M	V8	mmm[D_{2h}]	-

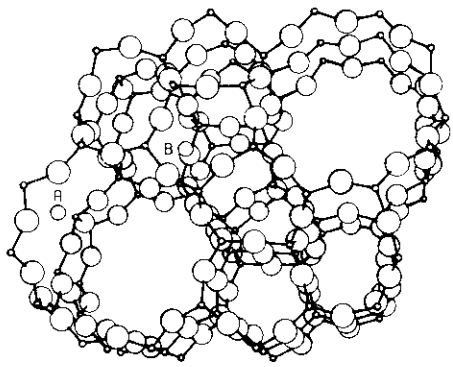
Site occupancies :

site :	A	B	C	D	E	F	G	H	I	J	K
(1)	1.8(K,Ba)	1.8(K,Ba)	1.2M	$2H_2O$	$4H_2O$	$1.8H_2O$	$4.8H_2O$	$1.6H_2O$	$1.6H_2O$	1M	1.6M

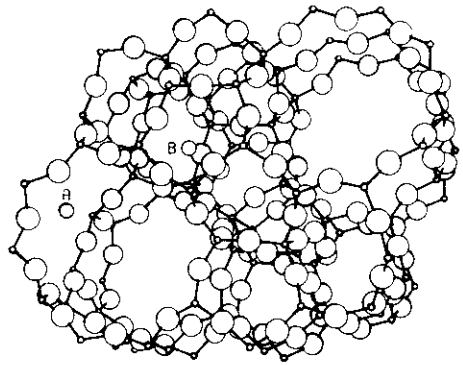
L	M
$3.2H_2O$	$0.4H_2O$

(1) $K_5Ca_2[9].24H_2O$; h; a = 14.12 b = 14.23 c = 9.95
E. Galli, G. Gottardi, D. Pongiluppi, Neues Jahrb. Miner. Mh., 1 (1979).

MFI



ZSM-5



ZSM-5

Framework MFI = $[Al_xSi_{96-x}O_{192}]$ $x < 27$ Pnma $V = 5306$ Å^3

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	V10	m[C_s]	-
B	V10	m[C_s]	-

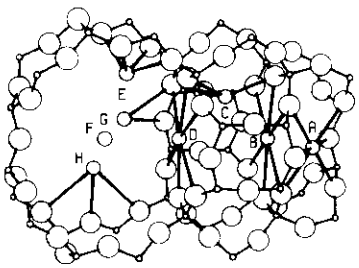
Site occupancies :

site :	A	B
(1)	-	-
(2)	1.5Ø	0.8Ø

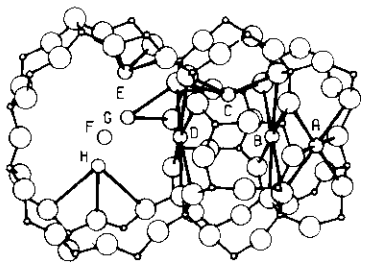
(1) [O]; calcined; $Pn2_1a$ a = 20.1 b = 19.8 c 13.4
[O, 1, 0, 0; 1/2, 0, 1, 0; 0, 0, 0, -1]
[Silica polymorph (SiO_2) with the same topology as ZSM-5]
E.M. Flanigen, J.M. Bennett, R.W. Grose, J.P. Cohen, R.L. Patton, R.M. Kirchner, J.V. Smith, Nature, 271, 512 (1978).

*(2) M_x[1.1]; h; a = 20.1 b = 19.9 c = 13.4
D.H. Olson, G.T. Kokotailo, L.S. Lawton, W.M. Meier, J. Phys. Chem., 85, 2238 (1981).

MOR



MORDENITE



MORDENITE

Framework MOR = $[Al_xSi_{48-x}O_{96}]$ x = 8 Cmcm V = 2794 $\mathring{A}^3$

Extra-framework sites :

site	type	site symmetry	coordination distances ($\mathring{A}$)
A	III8	$2/m[C_{2h}]$	2x2.54 4x2.83
B	III8	$mm[C_{2v}]$	2x3.19 4x3.25
C	IV8	1	2.58 2.66 2.80 2.88
D	III12	$mm[C_{2v}]$	2x3.04 4x3.30
E	IV12	$m[C_s]$	2x2.61 2x2.61
F	V12	$mm[C_{2v}]$	-
G	IV12	1	3.10 3.30
H	IV12	$2[C_2]$	2.84 2x3.37

Site occupancies :

site :	A	B	C	D	E	F	G	H
(1)	4Na	-	-	-	-	-	-	-
(2)	4Ø	4Ø	4Ø	4Ø	8Ø	1Ø	8Ø*	-
(3)	1.7Ca	-	0.6Ca*	0.5Ca*	0.6Ca	-	-	-
(4)	0.7Na	-	-	-	-	-	-	-
(5)	1.7Ca	$4H_2O$	$4.7H_2O$**	$3.4H_2O$	$8.7H_2O$	1.7Ca*	$10.3H_2O$	-
(6)a.	-	3.3K*	-	3.0K*	0.9K*	-	-	-
b.	1.9K	$4.5H_2O$*	$4.7H_2O$**	3.0K*	$5.8H_2O$	-	$8.4H_2O$	$6.5H_2O$
(7)a.	1.9Ca	-	0.6Ca	0.4Ca	0.5Ca	-	-	-
b.	2.0Ca	-	0.4Ca	0.7Ca	0.5Ca	-	-	-
c.	1.8Ca	-	0.5Ca	0.5Ca	0.6Ca	-	-	-
d.	2.1Ca	$2.6H_2O$	0.4Ca	0.1Ca	0.6Ca	-	-	-
(8)	-	3.7Rb*	-	3.1Rb	0.7Rb	-	-	-
(9)	0.3Ca	1.9Ba*	0.3Ba	1.1Ba	-	-	-	-
(10)	3.8Cs*	-	-	1.9Cs	1.8Cs	-	-	-
(11)	3.1Na*	-	-	2.6Na*	1.5Na*	-	-	-
(12)	0.6Na	-	-	-	-	-	-	-
(13)	1.4Ca	-	-	-	-	-	-	-

(1) $Na_8[8].24H_2O$; h; a = 18.13 b = 20.49 c = 7.52
W.M. Meier, Z. Kristallogr., 115, 439 (1961).

(2) $Na_8[8].24H_2O$; h; a = 18.11 b = 20.53 c = 7.53
V. Gramlich, Ph.D. thesis, ETH-Zürich (1971).

(3) $Ca_{3.3}$[7.8]; d; a = 18.01 b = 20.27 c = 7.47
W.J. Mortier, J.J. Pluth, J.V. Smith, Mat. Res. Bull., 10, 1037 (1975).

(4) $Na_{0.4}K_{0.1}H_x$[7.9]; d; a = 18.22 b = 20.47 c = 7.53
W.J. Mortier, J.J. Pluth, J.V. Smith, Mat. Res. Bull., 10, 1319 (1975).

(5) $Ca_{3.3}$[7.8].xH_2O; h; a = 18.12 b = 20.46 c = 7.52
W.J. Mortier, J.J. Pluth, J.V. Smith, Mat. Res. Bull., 11, 15 (1976).

(6) a. K_8[8]; d; Pbcn a = 18.03 b = 20.41 c = 7.46
b. K_8[8].xH_2O; h; a = 18.17 b = 20.61 c = 7.59
W.J. Mortier, J.J. Pluth, J.V. Smith in "Natural Zeolites", L.B. Sand and F.A. Mumpton, eds., Pergamon Press, 1978, p. 53.

(7) a. $Ca_{3.3}$[7.8]; d; a = 18.01 b = 20.25 c = 7.46
b. $Ca_{3.3}$[7.8]; d; a = 18.06 b = 20.33 c = 7.49
c. $Ca_{3.3}$[7.8]; d; a = 18.05 b = 20.28 c = 7.48
d. $Ca_{3.3}$[7.8]; d; a = 17.88 b = 20.19 c = 7.48
W.J. Mortier, J. Phys. Chem., 81, 1334 (1977).

(8) Rb_8[8]; d; a = 18.13 b = 20.41 c = 7.46
J.L. Schlenker, J.J. Pluth, J.V. Smith, Mat. Res. Bull., 13, 77 (1978).

(9) $Ca_{0.4}Ba_{3.3}$[8.6]; d; Pbcn a = 17.97 b = 20.32 c = 7.42
J.L. Schlenker, J.J. Pluth, J.V. Smith, Mat. Res. Bull., 13, 169 (1978).

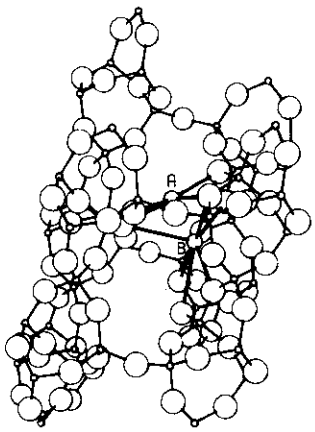
(10) $Cs_{7.4}$[8]; d; ($P2_1cn$?) a = 18.19 b = 20.47 c = 7.51
J.L. Schlenker, J.J. Pluth, J.V. Smith, Mat. Res. Bull., 13, 901 (1978).

(11) $Na_{7.3}K_{0.2}Ca_{0.0}$[8.3]; d; Pbcn a = 17.92 b = 20.31 c = 7.48
J.L. Schlenker, J.J. Pluth, J.V. Smith, Mat. Res. Bull., 14, 751 (1979).

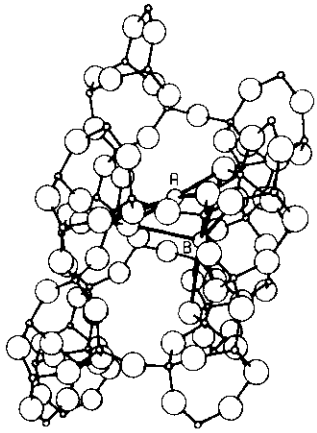
(12) $H_{8.4}$[8.4]; d; a = 18.18 b = 20.39 c = 7.49
J.L. Schlenker, J.J. Pluth, J.V. Smith, Mat. Res. Bull., 14, 849 (1979).

(13) $Na_{0.2}K_{0.1}Ca_{1.8}H_x$[8.5]; d; a = 18.06 b = 20.30 c = 7.48
J.L. Schlenker, J.J. Pluth, J.V. Smith, Mat. Res. Bull., 14, 961 (1979).

NAT



NATROLITE



NATROLITE

Framework NAT = $[Al_xSi_{40-x}O_{80}]$ x = 16 Fdd2 V = 2250 $Å^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)						
A	III8	1	2.4	2.4	2.5	2.6			
B	III8	1	2.9	3.0	3.3	3.3	3.4	3.4	3.5

Site occupancies :

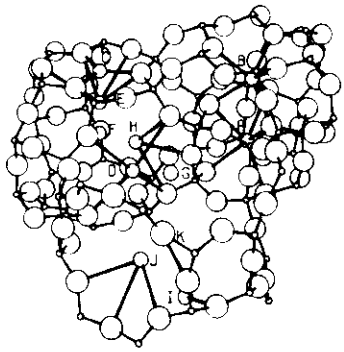
site :	A	B
(1)	-	-
(2)	16Na	$16H_2O$
(3)	16Na	$16H_2O$
(4)	16Na	$16H_2O$

(1) Na_{16}[16].$16H_2O$; h; a = 18.19 b = 18.62 c = 6.58
L. Pauling, Proc. Natl. Acad. Sci., 16, 453 (1930).

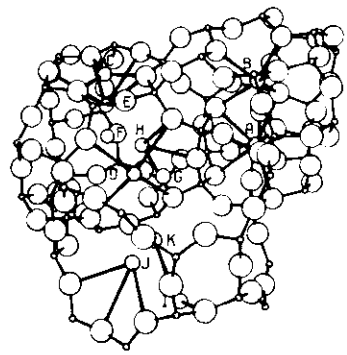
(2) Na_{16}[16].$16H_2O$; h; a = 18.30 b = 18.60 c = 6.57
W.H. Taylor, C.A. Meek, W.W. Jackson, Z. Kristallogr., 84, 373 (1933).

(3) Na_{16}[16].$16H_2O$; h; a = 18.30 b = 18.63 c = 6.60
W.M. Meier, Z. Kristallogr., 113, 430 (1960).

(4) Na_{16}[16].$16H_2O$; h; a = 18.30 b = 18.63 c = 6.60
[protons located.]
B.H. Torrie, I.D. Brown, H.E. Petch, Can. J. Phys., 42, 229 (1964).



OFFRETITE



OFFRETITE

Framework OFF = $[Al_xSi_{18-x}O_{36}]$ x = 4 $P\bar{6}m2$ V = 1112 $Å^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	I	$\bar{6}m2[D_{3h}]$	6x2.9
B	II6	$\bar{6}m2[D_{3h}]$	6x2.6
C	II8	$\bar{6}m2[D_{3h}]$	3x2.1
D	III12	$mm[C_{2v}]$	2x3.3 2x3.3
E	II8	$3m[C_{3v}]$	3x2.8 3x3.4
F	V8	$\bar{6}m2[D_{3h}]$	-
G	V12	$3m[C_{3v}]$	-
H	IV8	$m[C_s]$	3.0 2x3.1
I	IV12	$m[C_s]$	3.2
J	IV12	$m[C_s]$	2x3.1 3.4
K	IV12	$m[C_s]$	3.3

Site occupancies :

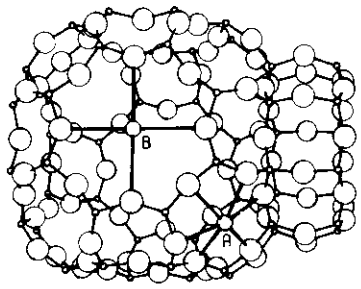
site :	A	B	C	D	E	F	G	H	I	J	K
(1)	0.1Ca*	1K	-	-	$1.8H_2O$	0.8Mg	0.8Ca*, $0.6H_2O$*	$1H_2O$*, $0.8H_2O$*	$1.7H_2O$	$2.8H_2O$	$1H_2O$
(2)	-	1Ca	0.7Mg	1K	-	-	-	-	-	-	-
(3)	-	1Ca	0.9Mg	1K	0.9C	0.9Ø	-	-	-	-	-

(1) $K_{1.1}Ca_{1.1}Mg_{0.7}[5.2].15.2H_2O$; h; a = 13.29 c = 7.58
J.A. Gard, J.M. Tait, Acta Crystallogr., B28, 825 (1972).

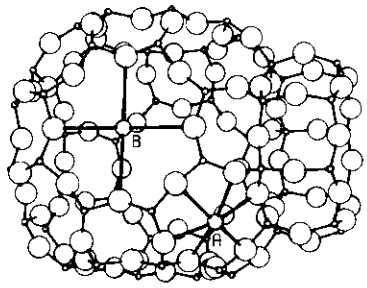
(2) $K_{1.0}Ca_{1.0}Mg_{1.0}[5.2]$; d; a = 13.23 c = 7.34
W.J. Mortier, J.J. Pluth, J.V. Smith, Z. Kristallogr., 143, 319 (1976).

(3) $K_{1.0}Ca_{1.0}Mg_{1.0}[5.2].xCO$; d+CO; a = 13.26 c = 7.35
W.J. Mortier, J.J. Pluth, J.V. Smith, Z. Kristallogr., 144, 32 (1976).

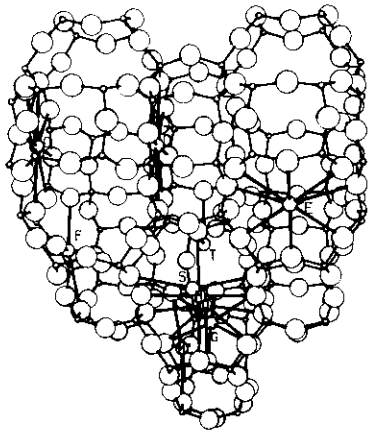
PAU



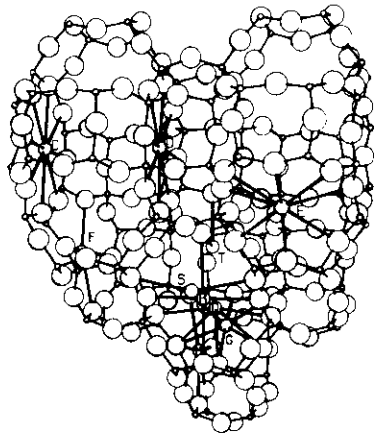
PAULINGITE-A



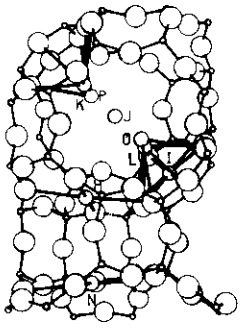
PAULINGITE-A



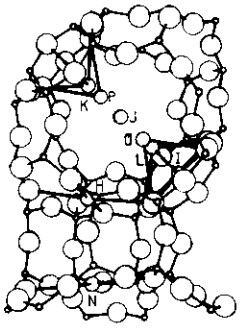
PAULINGITE-B



PAULINGITE-B



PAULINGITE-C



PAULINGITE-C

Framework PAU = $[Al_xSi_{672-x}O_{1344}]$ x = 152 Im3m V = 43218 $Å^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)				
A	II8	$3m[C_{3v}]$	3x2.56	3x2.69			
B	III8	$4mm[C_{4v}]$	4x3.28				
C	III8	$4mm[C_{4v}]$	4x3.40	4x3.44			
D	III8	$4mm[C_{4v}]$	4x3.34	4x3.48			
E	III8	$m[C_s]$	2x2.89	2x3.22	2x3.25	3.43	3.49
F	III8	$m[C_s]$	2x2.93	2x3.37			
G	III8	$mm[C_{2v}]$	2x2.87	4x3.23			
H	III8	$m[C_s]$	2x3.00	2x3.25			
I	II8	$\bar{3}m[D_{3d}]$	6x2.59				
J	V8	$3m[C_{3v}]$	-				
K	II8	$3m[C_{3v}]$	3x3.00	3x3.50			
L	II8	$3m[C_{3v}]$	3x3.04	3x3.50			
M	III8	$m[C_s]$	2x3.10	3.24	2x3.26		
N	III8	$m[C_s]$	3.11	3.15	2x3.29		
O	IV8	$m[C_s]$	2x3.14				
P	IV8	$m[C_s]$	2x3.20				
Q	IV8	$m[C_s]$	3.21	2x3.33	2x3.40		
R	III8	$m[C_s]$	2x3.00	3.37	3.45		
S	IV8	$mm[C_{2v}]$	2x3.25				
T	IV8	$mm[C_{2v}]$	2x2.91				

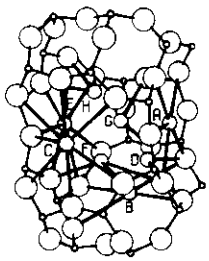
Site occupancies :

site :	A	B	C	D	E	F	G	H	I	J
(1)	-	xH_2O	xH_2O	xH_2O	48M	-	24M	$48H_2O$	-	16M
	K	L	M	N	O	P	Q	R	S	T
	$16H_2O$	$16H_2O$	$48H_2O$	$48H_2O$	xH_2O	xH_2O	xH_2O	xH_2O	xH_2O	xH_2O

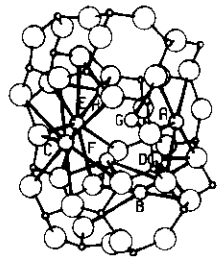
(1) $K_{68}Ca_{36}Na_{13}Ba_2[152].705H_2O$; h; a = 35.09
E.K. Gordon, S. Samson, W.B. Kamb, Science, 154, 1004 (1966).
M = K, Ca, Ba.

NOTE : Each one of the three stereo plots displays only one part of the complicated Paulingite framework. They are chosen such that each contains the type of cage denoted as the A-cage, B-cage and C-cage respectively.

PHI



PHILLIPSITE



PHILLIPSITE

Framework PHI = $[Al_xSi_{16-x}O_{32}]$ x = 5 $P2_1/m$ V = 1012 $Å^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	III8	m[C_s]	4x3.03 3.27
B	III8	$\bar{1}$[C_i]	2x2.32 2x2.86
C	III8	m[C_s]	2x2.95 2x3.13 2x3.37 3.43
D	IV8	1	2.51 2.58 2.60
E	III8	m[C_s]	2x3.15 3.29 2x3.32 2x3.43
F	IV8	1	2.94 3.29 3.47
G	IV8	m[C_s]	2x3.14
H	IV8	1	2.42 2.76

Site occupancies :

site :	A	B	C	D	E	F	G	H
(1)	$2H_2O$	$2H_2O$*	2Ba	-	$2H_2O$	$2H_2O$	$2H_2O$*	-
(2)	$2H_2O$	-	4Na, K	$4H_2O$, Na	$2H_2O$	$4H_2O$	$4H_2O$, $2H_2O$***	$4H_2O$
(3)	$2.2H_2O$	$2.5H_2O$	0.9K, 1.1K	1.6Ca	$2.1H_2O$	$4.2H_2O$	$2.4H_2O$	-
(4)a.	$2H_2O$	$2H_2O$	2K	1.7Ca	$2H_2O$	$4H_2O$	$2H_2O$	-
b.	$2H_2O$	$2H_2O$	2Ba	0.6Ca	$2H_2O$	$4H_2O$	$2H_2O$	-

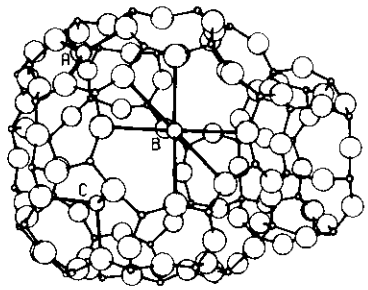
(1) Ba_2[4].$12H_2O$; h; $P2_1$ a = 9.87 b = 14.14 c = 8.72 β = 124.8°
R. Sadanaga, F. Masumo, Y. Takéuchi, Acta Crystallogr., 14, 1153 (1961).

(2) $(K,Na)_{10}$[2x5].$20H_2O$; h; B2mb a = 9.96 b = 14.25 c = 14.25
[0, 1, 0, 1; 0, 0, 1, 0; 1/2, 0, 0, 2]
H. Steinfink, Acta Crystallogr., 15, 644 (1962).

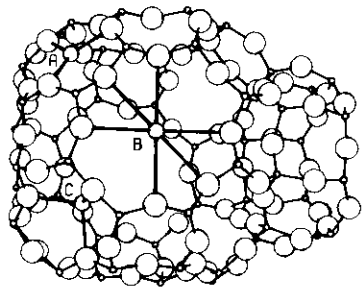
(3) $K_2Ca_{1.7}Na_{0.4}$[5.3].$13.5H_2O$; h; a = 9.87 b = 14.3 c = 8.67 β = 124.2°
R. Rinaldi, J.J. Pluth, J.V. Smith, "Molecular Sieves", J.B. Uytterhoeven, ed., Proc. Third Int. Conf. Mol. Sieves, p. 100 (1973).

*(4) a. $K_2Ca_{1.5}Na_{0.4}$[5].$12H_2O$; h; a = 9.87 b = 14.3 c = 8.67 β = 124.2°
b. $Ba_2Ca_{0.5}$[5].$12H_2O$; h; a = 9.88 b = 14.14 c = 8.69 β = 124.8°
R. Rinaldi, J.J. Pluth, J.V. Smith, Acta Crystallogr., B30, 2426 (1974).

RHO



RHO



RHO

Framework RHO = $[Al_xSi_{48-x}O_{96}]$ x = 12 $I\bar{4}3m$ V = 3443 $\AA^3$

Extra-framework sites :

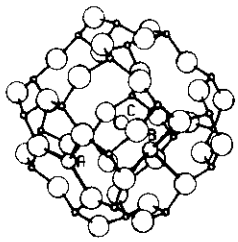
site	type	site symmetry	coordination distances (Å)
A	II8	$3m[C_{3v}]$	3x2.3
B	III8	$\bar{4}2m[D_{2d}]$	2x3.3 4x3.3
C	II8	$3m[C_{3v}]$	3x2.5

Site occupancies :

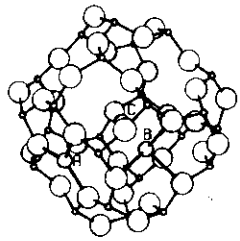
(1) no cations or water molecules located.

(1) $Na_{9.6}Cs_{3.0}[12.3].xH_2O$; h; a = 15.0
H.E. Robson, D.P. Shoemaker, R.A. Ogilvie, P.C. Manor, Adv. Chem. Ser., 101, 106 (1973).

SOD



SODALITE



SODALITE

Framework SOD = $[Al_xSi_{12-x}O_{24}]$ x = 6 $P\bar{4}3n$ V = 700 $Å^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	II6	3[C_3]	3x2.1
B	II6	3[C_3]	3x2.4
C	V6	23[D_3]	-

Site occupancies :

site :	A	B	C
(1)	-	8Na	2Cl
(2)a.	-	8Na, 4Ø	S
b.	-	8Na, 4Ø	W
(3)a.	x(Na,Ca)	x(Na,Ca)	xS
b.	x(Na,Ca)	x(Na,Ca)	xS
(4)	3.6Na	3.4Na	S
(5)	-	8Na	-
(6)	-	8Na::	2Cl
(7)	-	8Na	2Cl
(8)	0.7H	0.7Ø, 7.1Na	0.4Cl
	+ positions of 2H replacing Si		
(9)	-	2.7Na, 0.8K, 0.8Ca, 2.4Na, 1.5Na	2S, 1.3Ø::::, 1.7Ø::
(10)	-	-	2N, 4C::::, 4C::::
(11)	-	8Ca	2Ø

(1) Na_8[6].2Cl; h; a = 8.87
L. Pauling, Z. Kristallogr., 74, 213 (1930).

(2) a. Na_8[6].SO_4; h; $P\bar{4}3m$ a = 9.05
b. Na_8[6].WO_4; h; $P\bar{4}3m$ a = 9.19
H. Saalfeld, Neues Jahrb. Mineral. Monatsh., 38 (1959).

(3) a. $(Ca,Na)_{4-8}$[6].$(SO_4)_{1-2}$; h;
b. $(Ca,Na)_{4-8}$[6].$(SO_4)_{1-2}$; h;
H. Saalfeld, Z. Kristallogr., 115, 132 (1961).

(4) Na_8[6].SO_4; d; $P\bar{4}3m$
H. Schulz, H. Saalfeld, Tschermaks Min. Petr. Mitt., 10, 225 (1965).

(5) Na_6[6].3.5H_2O; h; a = 8.88
T.N. Shishakova, M.M. Dubinin, Izv. Akad. Nauk. SSSR, Ser. Khim., 1303 (1965).

(6) Na_8[2+2Be].2(Cl,S); h; $I\bar{4}$ a = 8.58 c = 8.82
M. Dano, Acta Crystallogr., 20, 812 (1966).

(7) $Na_8[6].Cl$; h; a = 8.87
H. Löns, H. Schulz, Acta Crystallogr., 23, 434 (1967).

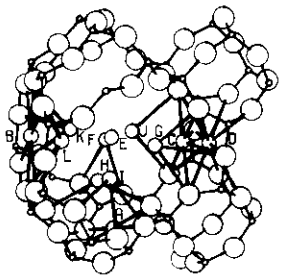
(8) $Na_6[6+2H].4NaCl.7NaOH$; h; a = 8.89
V.I. Bukin, Ye.S. Makarov, Geochem. Intern., 4, 19 (1967).

(9) $Na_5KCa_2[6].1.5SO_4$; h; a = 9.12
J. Löhn, H. Schulz, Neues Jahrb. Mineral. Abh., 109, 201 (1968).

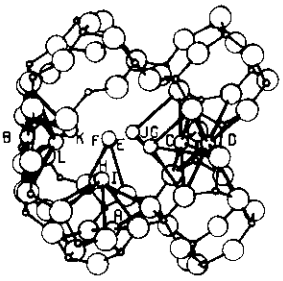
(10) $((CH_3)_4N)_2[2]$; h; I23 a = 8.98
Ch. Baerlocher, W.M. Meier, Helv. Chim. Acta, 52, 1853 (1969).

(11) $Ca_8[12].2Ø$; d; $I\bar{4}3m$ a = 8.86
V.I. Ponomarev, D.M. Kheiker, N.V. Belov, Kristallografiya, 15, 918 (1970).

STI



STILBITE



STILBITE

Framework STI = $[Al_xSi_{36-x}O_{72}]$ x = 10 c2/m V = 2220 $Å^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)
A	II10	$\bar{1}[C_i]$	2x2.2 2x2.8
B	III10	$2/m[C_{2h}]$	2x2.8 4x3.2
C	III10	$m[C_s]$	2.7 2x2.9 2x2.9 2.9
D	III10	$2/m[C_{2h}]$	2x2.5 4x3.2 4x3.2
E	V10	$m[C_s]$	-
F	IV10	$2[C_2]$	2x3.0
G	IV10	$m[C_s]$	2x2.9 3.5
H	IV10	1	3.0 3.0 3.3
I	IV10	1	2.9 3.1 3.5
J	IV10	$m[C_s]$	2x3.2
K	IV10	$m[C_s]$	2x3.1 3.4
L	IV10	$m[C_s]$	2x3.0 2x3.2

Site occupancies :

site :	A	B	C	D	E	F
(1)	-	-	-	-	4Ca	-
(2)	-	0.2X※※	-	0.3Na※	3.4Ca, 0.6Na	1.6Na※
(3)	-	-	-	-	4Ca	1.8Na※
(4)	-	-	-	-	8Ca	$6.4H_2O$※※
(5)	-	2.0M	$2H_2O$, $2H_2O$	-	2.9M, 2.4M	2.2M
(6)a.	-	-	3.0M	-	$3.4H_2O$※※	2.2M
b.	-	$2.6H_2O$	1.9M	-	$3.4H_2O$※※ $3.0H_2O$ $2.6H_2O$	1.8M
(7)	-	1.1Ca	1.5Ca	-	-	-

Site occupancies : continued.

site :	G	H	I	J	K	L
(1)	-	-	-	-	-	-
(2)	$3.5H_2O$	$6.6H_2O$	$5.2H_2O$	$3.3H_2O$*	$2.6H_2O$	$0.2Na$* $3.4H_2O$
(3)	$4H_2O$	$7.3H_2O$	$6.7H_2O$	$4H_2O$	$4H_2O$	$3.4H_2O$
(4)	$6.9H_2O$ $9.9H_2O$	$6.4H_2O$ $12.8H_2O$	-	-	$7.2H_2O$	$5.9H_2O$
(5)	$1.6H_2O$ $6.6H_2O$	$7.8H_2O$, $2.3H_2O$ $7.3H_2O$	4.0M $6.6H_2O$	$3.4H_2O$***, $4H_2O$	$3.0H_2O$*** $4.0H_2O$	$3.7H_2O$ $4.0H_2O$***
(6)a.	$0.8H_2O$***	8Ø***	2.6M***	1.9M***	$1.1H_2O$	0.6M*** $1.4H_2O$***
b.	$3.9H_2O$***	8Ø***, $3.3H_2O$	1.5M*** $3.1H_2O$***	2.2M***	$1.8H_2O$	3.4M*** $2.8H_2O$*** $2.8H_2O$***
(7)	-	-	-	-	-	-

(1) Na_2Ca_4[10].$28H_2O$; h; a = 13.6 b = 18.2 c = 11.3 β = 128°
E. Galli, G. Gottardi, Miner. Petrogr. Acta, 12, 1 (1966).

(2) Na_3Ca_3[10].$25H_2O$; h; a = 13.7 b = 18.3 c = 11.3 β = 128°
M. Slaughter, Amer. Mineral., 55, 387 (1970).

(3) Na_1Ca_4[10].$34H_2O$; h; a = 13.6 b = 18.2 c = 11.3 β = 128°
E. Galli, Acta Crystallogr., B27, 833 (1971).

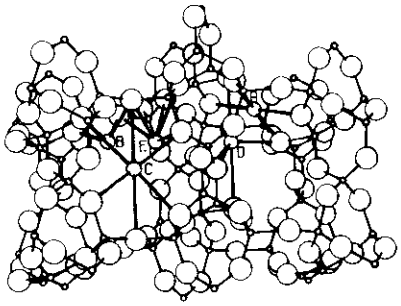
(4) $Ca_{7.6}Mg_{0.1}Na_{0.3}K_{0.3}$[2x7.9].$56.2H_2O$; Fmmm a = 13.60 b = 18.22 c = 17.86
[0, -1, 0, 1; 0.5, 0, -1, 0; 0.5, 0, 0, 2]
E. Galli, A. Alberti, Bull. Soc. Fr. Mineral. Crystallogr., 98, 11 (1975).

(5) $Ca_{1.7}Mg_{0.3}Na_{10.9}K_{2.1}$[2x8.2].$51.6H_2O$; Amma a = 13.64 b = 18.20 c = 17.84
[0, -1, 0, 1; 0.5, 0, -1, 0; 0, 0, 0, 2]
E. Galli, A. Alberti, Bull. Soc. Fr. Mineral. Crystallogr., 98, 331 (1975).

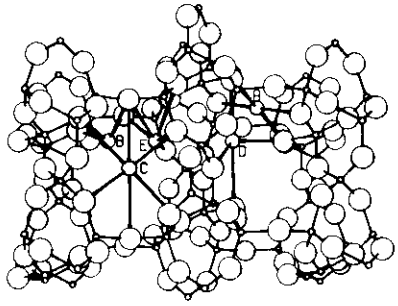
(6) a. $Ca_{1.7}Mg_{0.3}Na_{10.9}K_{2.1}$[2x8.2].$xH_2O$; d; Amma a = 13.61 b = 17.12 c = 16.03
[0, -1, 0, 1; 0.5, 0, -1, 0; 0, 0, 0, 2]
b. $Ca_{1.7}Mg_{0.3}Na_{10.9}K_{2.1}$[2x8.2].$xH_2O$; d; Amma a = 13.61 b = 17.61 c = 16.24
[0, -1, 0, 1; 0.5, 0, -1, 0; 0, 0, 0, 2]
A. Alberti, G. Vezzalini, "Natural Zeolites", L.B. Sand and F.A. Mumpton, eds., Pergamon Press, p. 85, (1978).

(7) $Na_1K_1H_8$[10]; d; a = 13.6 b = 18.2 c = 11.3 β = 127°
J.R. Pearce, W.J. Mortier, G.S.D. King, J.J. Pluth, I.M. Steele, J.V. Smith, Proc. Vth Int. Conf. Zeolites, Naples 1980, L.V.C. Rees, ed., Heyden, London, p. 261, (1980).

THO



THOMSONITE



THOMSONITE

Framework THO = $[Al_xSi_{20-x}O_{40}]$ x = 10 Pbmn V = 1130 $Å^3$

Extra-framework sites :

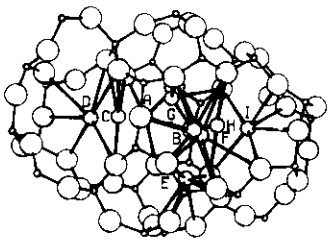
site	type	site symmetry	coordination distances (Å)
A	III8	$2/m[C_{2h}]$	2x2.1 4x3.1
B	IV8	$m[C_s]$	2x2.3 2x2.6
C	III8	$2[C_2]$	2x2.8 2x3.3 2x3.4
D	IV8	$m[C_s]$	2.6 2x2.8 2x3.3
E	IV8	$m[C_s]$	2.6 2x2.9 2x3.1

Site occupancies :

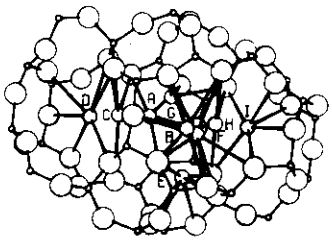
site :	A	B	C	D	E
(1)	2Ca	4(Ca,Na)	$4H_2O$	$4H_2O$	$4H_2O$

(1) $Na_2Ca_4[10].12H_2O$; h; a = 13.07 b = 13.09 c = 6.61
W.H. Taylor, C.A. Meek, W.W. Jackson, Z. Kristallogr., 84, 373 (1933).

YUG



YUGAWARALITE



YUGAWARALITE

Framework YUG = $[Al_xSi_{16-x}O_{32}]$ x = 4 Pc V = 876 $\AA^3$

Extra-framework sites :

site	type	site symmetry	coordination distances (Å)					
A	III8	1	2.44	2.48	2.50	2.50		
B	III8	1	2.20	2.60	2.71	3.00	3.33	
C	IV8	1	2.85	3.30	3.31	3.44		
D	IV8	1	2.87	3.11	3.14	3.25	3.27	3.30
E	IV8	1	1.87 3.31	2.68	2.75	2.87	2.94	3.04
F	IV8	1	2.91 3.35	3.15	3.16	3.21	3.25	3.29
G	IV8	1	2.90	2.91	3.12	3.31		
H	IV8	1	2.89	3.07	3.20	3.37		
I	III8	1	2.91	3.12	3.18	3.22	3.28	3.36

Site occupancies :

site :	A	B	C	D	E	F	G	H	I
(1)	2Ca	-	-	-	-	-	-	-	-
(2)	2Ca	-	$1.5H_2O$	-	-	$2H_2O$	$1.5H_2O$	-	$1.5H_2O$
(3)	1.2Ca	0.8Ca	$1.6H_2O$	$1.4H_2O$	$0.3H_2O$	$1.2H_2O$	$2H_2O$	$0.8H_2O$	$0.5H_2O$

(1) $Ca_2[4].8H_2O$; h; a = 6.73 b = 13.95 c = 10.03 β = 111.5°
I.S. Kerr, D.J. Williams, Z. Kristallogr., 125, 220 (1967).

(2) $Ca_2[4].8H_2O$; h; a = 6.73 b = 13.95 c = 10.03 β = 111.5°
I.S. Kerr, D.J. Williams, Acta Crystallogr., B25, 1183 (1969).

(3) $Ca_2[4].8H_2O$; h; a = 6.73 b = 13.96 c = 10.02 β = 11.5°
H.W. Leimer, M. Slaughter, Z. Kristallogr., 130, 88 (1969).