### ERMANNO GALLI\*

# CRYSTAL STRUCTURE REFINEMENT OF MAZZITE \*\*

RIASSUNTO. — La mazzite, Nano. K2. 5Ca1. 4Mg2.1 [Alg. 6Size. 5O72] · 28H2O, probabile corrispondente naturale della zeolite  $\Omega$ , cristallizza nel sistema esagonale con a = 18,392 e c = 7,646 Å. La sua struttura è stata raffinata nel gruppo spaziale  $P6_s/mmc$  fino ad un R = 0,049 per i 681 riflessi osservati. L'impalcatura è caratterizzata dalla presenza di gabbie tipo gmelinite che si sovrappongono dando luogo a colonne parallele a c. Queste, sfasate di c/2 per la presenza di uno slittopiano, sono legate lateralmente tra di loro e delimitano due tipi di canali, pure paralleli a c. I cationi scambiabili sono distribuiti in tre posizioni diverse: il Mg++, completamente circondato da acqua, è posto al centro delle cavità tipo gmelinite; gli ioni (K+, Na+, Ca++), legati sia ad ossigeni dell'impalcatura sia a molecole d'acqua, si trovano nelle cavità tra le gabbie; il Ca++ completamente circondato da molecole d'acqua, si trova al centro dei grandi canali delimitati da anelli di 12 tetraedri.

ABSTRACT. - Mazzite, Na<sub>N0.8</sub>K2.6Ca1.4Mg2.1[Als.6Si28.8Or2].28H2O, probably the natural counterpart of the synthetic zeolite  $\Omega$ , crystallizes in the hexagonal system with a = 18.392and c = 7.646 Å. Its crystal structure was refined in the space group P6<sub>3</sub>/mmc to a residual R of 0.049 for the 681 observed reflections. The alumino-silicate framework consists of gmelinite-type cages superimposed to form columns parallel to c. The columns, shifted by c/2in accord with a c glide plane, are cross-linked to form two different types of channels parallel to c. The exchangeable cations are distributed into three positions: Mg++ is completely surrounded by water molecules in the gmelinite-type cages; (K<sup>+</sup>, Na<sup>+</sup>, Ca<sup>++</sup>) ions are coordinated both to framework oxygens and water molecules between the cages; and Ca<sup>++</sup> is completely surrounded by water molecules in the middle of the largest channels formed by rings of 12-tetrahedra.

### Introduction

The zeolite, mazzite described as a new mineral by GALLI et al. (1974), is closely related to the synthetic molecular sieve  $\Omega$  (UNION CARBIDE Co., 1967); they probably have the same framework.

The present study was undertaken to determine the details of the crystal structure of mazzite, and to compare it with the structure proposed by BARRER and  $V_{ILLIGER}$  (1969) for molecular sieve  $\Omega$ . A preliminary report on the structure determination was published elsewhere (GALLI, 1974). The crystal structure of mazzite dehydrated at 600° C has been recently described (RINALDI et al., 1975).

<sup>\*</sup> Istituto di Mineralogia e Petrologia dell'Università di Modena.

<sup>\*\*</sup> Paper presented at the Ninth General Meeting of the International Mineralogical Association. September 1974, Berlin-Regensburg, Germany.

#### E. GALLI

#### Experimental

A regular hexagonal prism, ca 0.6 mm long and 0.04 mm wide, was removed from the holotype of GALLI et al. (1974) from Mont Semiol, Montbrison, Loire, France, the original locality for offretite. It was mounted parallel to the elongation (*c*-axis). Unit cell dimensions obtained with a 4-circle automatic diffractometer agree with those accurately determined by GALLI et al. (1974) from powder diffractometry:

### $a = 18.392 \pm 0.008$ , $c = 7.646 \pm 0.002$ A

The systematically absent reflections (l odd in hh $\overline{2}$ hl) indicate P6<sub>3</sub>/mmc, P $\overline{6}$ 2c or P6<sub>3</sub>mc as possible space-groups.

Chemical analysis from new electron probe data (RINALDI et al., 1975) yielded a unit cell content of:

### $Na_{N0.3}K_{2.5}Ca_{1.4}Mg_{2.1}[Al_{9.9}Si_{26.5}O_{72}] \cdot 28H_2O$

Intensity data were collected with a Picker FACS-1 automatic four-circle diffractometer of the Department of the Geophysical Sciences of the University of



Fig. 1. — Structural scheme for the  $\alpha$  gmelinite-type » cage. T atoms lie at the intersections and the O-atoms near the mid-points of each line.

Chicago with  $\vartheta$ -2 $\vartheta$  scans (1° min<sup>-1</sup>) using Cuk $\alpha$  radiation ( $\lambda = 1.5418$  Å). Four sets of equivalent diffraction (sin  $\vartheta/\lambda_{max} = 0.562$ ) were averaged to 759 independent reflections, of which 78 were considered to be unobservable, having  $F_0 \leq 2\sigma_{F0}$ . Data processing was carried out in the manner described by RINALDI et al. (1975) to yeld  $|F_0|$  and  $\sigma|_{F^0}|$ . No correction for absorption was applied because of the low absorption coefficient and the small dimensions of the crystal.

Some difficulties were experienced during data collection due to instability of the intensities of the standard diffractions. This problem was overcome by applying at the free end of the crystal a second drop of epoxy resin, similar to that used to fix it on the side of the goniometer head. Perhaps water molecules were moving in response to changes of relative humidity and the epoxy sealed the one-dimensional channel system. The structure was solved starting from the «gmelinite-type» cage (Fig. 1) which was assumed by BARRER and VILLIGER (1969) to be part of the structure of zeolite  $\Omega$ . Space group P6<sub>3</sub>/mmc requires that the cages be staggered by c/2, whereas BARRER and VILLIGER (1969) placed all of them at the same height. Refinement of F's was carried out with a modified ORFLS full-matrix least-squares



Fig. 2. - The superimposing and cross linking of «gmelinite-type cages» in the mazzite structure, represented as in Fig. 1. Atoms are coded as in Table 1.

program (BUSING et al., 1962) and by Fourier syntheses. Atomic scattering factors (CROMER and MANN, 1968) were used for Mg<sup>++</sup>, K<sup>+</sup>, Ca<sup>++</sup>, Na<sup>+</sup> and [1/4 Al<sup>+</sup> + 3/4 Si<sup>++</sup>] (for which Al<sup>+</sup> was interpolated between Al and Al<sup>3+</sup> and Si<sup>++</sup> between Si and Si<sup>4+</sup>). The final model, checked by difference Fourier synthesis, did not show any significant residual electron density. Attempts to refine the structure in P62c and P63mc resulted in worse R values than for the centric space-group. The lowest R-value (R =  $\Sigma$  ||Fo-Fc|/ $\Sigma$ |Fo|) with framework atoms only was 0.37. Introduction of exchangeable cations and water molecules (detected with three dimensional electron density maps) resulted in R = 0.075 with isotropic temperature factors. Partial anisotropic refinement on all atoms excluding Ca in

602

Atom S	ymmetry	* x/a	y/ <u>b</u>	z/ <u>c</u> / 5	ll <sup>or B(Å)</sup>	- <sup>2</sup> /5 22	/ <b>3</b> 33	$\beta_{12}$	/ <sup>3</sup> 13	$\beta_{23}$	¢ccupanc
T(1)	12(j)	.1584 (1)	.4902(1)	1/4	9(1)	9(1)	60(3)	5(1)	0	0	100
T(2)	24(1)	.3536(1)	.0933(1)	.0444(2)	10(1)	7(1)	59(2)	4(1)	2(1)	-0(1)	100
0(1)	6(h)	.2589(2)	.5178	1/4	14(2)	20(4)	166(18)	10	0	0	100
0(2)	6(h)	.4249(2)	.8498	1/4	14 (2)	16(3)	116(16)	8	0	0	100
0(3)	12(j)	.3822(3)	.1004(3)	1/4	24 (2)	27(3)	78(9)	17(2)	0	0	100
0(4)	24 (1)	.4352(2)	.1114(2)	0721(5)	21(2)	25(2)	106(8)	14(1)	9(3)	8(3)	100
0(5)	12(k)	.1614(2)	.3228	<b></b> 0016(6)	14(1)	22(2)	107(11)	11	4(2)	000	100
0(6)	12(i)	.2741(3)	0	0	20(2)	12(2)	153(14)	6	-3(2)	-6	100
K,Na,Ca	6(g)	1/2	0	0	19(2)	30(3)	217(17)	15	20(3)	40	50(1)
Mg	2(d)	1/3	2/3	-1/4	32(2)	32	93 (14)	16	0	0	100
Са	4(e)	0	0	•072(8)	23.2(32	<b>`</b>		÷			22(1)
H,0(1)	12(k)	.467(1)	•934	.661(2)	6.4(4)						50(1)
$H_{2}^{-0}(2)$	4(f)	1/3	2/3	.016(1)	$4 \cdot 3(3)$						100
H,0(3)	6(h)	.271(1)	• 54 2	-1/4	5.4(6)						44
$H_{2}^{2}0(4)$	12(j)	.566(1)	•355(1)	1/4	6.9(5)						44
н,0(5)	24 (1)	.028(2)	.148(1)	•030(4)	7.7(11)	Ū					23(1)
H,0(6)	6(h)	.088(1)	.176	1/4	21.8(19)	Ū					89(5)
H <sup>2</sup> <sub>2</sub> 0(7)	6(h)	.076(1)	.152	-1/4	31.2(30)	•					45(3)
1											

Atomic coordinates, thermal parameters and occupancy factors with e.s.d.'s on the last digit in parentheses. The form of the anisotropic temperature factors  $(x \ 10^4)$  is:  $exp[--(h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23})]$ 

TABLE 1

;

Atom I	Principal axis	R.m.s. amplitude	$\vartheta_{_1}$	$\vartheta_2$	ୢୄୢ୰
	1	.10(1)	28(40)°	62(40)°	90 <b>°</b>
T(1)	2	.11(1)	118(40)	28 (40)	90
	3	.13(1)	90	90	0
	1	.09(1)	101(6)	169(6)	93(4)
T(2)	2	.12(1)	160(7)	79(6)	107(7)
	3	.13(1)	73(7)	90(4)	163(7)
	1	.12(4)	0	90	90
0(1)	2	.16(2)	90	0	90
	3	.22(1)	90	90	0
	1	.13(2)	0	90	90
0(2)	2	.15(1)	90	0	90
	3	.19(1)	90	90	0
	1	.15(1)	21(9)	69(9)	90
0(3)	2	.15(1)	90	90	0
	3	.19(1)	69(9)	159(9)	90
	1	.15(1)	22(13)	91 (13)	68 (13)
0(4)	2	.17(1)	74 (16)	42(9)	128(12)
	3	.19(1)	74(7)	132(9)	133(8)
	1	.12(1)	0	90	90
0(5)	2	.15(1)	90	33(12)	123(12)
	3	.19(1)	90	123(12)	147(12)
	1	.13(2)	<b>90</b> ·	172(5)	98(5)
0(6)	2	.17(2)	0	90	90
	3	.21(1)	90	82(5)	172(5)
	1	.14(1)	0	90	90
K,Na,(	Ca 2	.15(1)	90	31(3)	121(3)
	3	.28(1)	90	121(3)	149(3)
	1	.17(1)	90	90	0
Mg*	2	.20(1)			
	3	.20			

Analisys of anisotropic thermal parameters. Root mean square thermal vibrations (Å)
along the ellipsoid axes and angles (°) between the principal axes (Ui) of the
vibration ellipsoid and the [100], [120] and [001] directions

\* Being a rotation ellipsoid, only the angles relative to the rotation axis are given.

TABLE 2

603

the large channels and all water molecules, converged to a final R = 0.049 (omitting zeros) and R = 0.054 (including zeros). The weighted Rw ( $Rw = [\Sigma w ||Fo-Fc||^2 / \Sigma w |Fo|^2]^{1/2}$  where  $w = (1/\sigma_{Fo})^2$ ) was 0.052.

Population refinement of H<sub>2</sub>O(3) and H<sub>2</sub>O(4) showed anomalously high values  $(54 \pm 3 \%)$  which were consequently held fixed at 44 % in accordance with statistical occupancy of geometrically related positions. In the last stages of the refinement the position of H<sub>2</sub>O(7) was held fixed at z/c = -1/4 after it had refined to a value of z/c = -264(14).

Positional and thermal atomic parameters are given in Table 1 and 2. The observed and calculated structure factors are listed in Table 3. Tables 4 and 5 contain the interatomic distances.

#### Structure refinement and discussion

Description of the structure may begin with the  $\epsilon$  gmelinite cage  $\ast$ , which is represented clinographically in Fig. 1; in this Figure each nodal point represents a tetrahedral-atom, oxygens being placed near the midpoint of the lines so that each line represents a T-O-T bridge. These cages are superimposed to build columns parallel to c, with the upper and the lower hexagonal rings in common between cages. Adjacent columns of cages are shifted by c/2 and interconnected as shown in Fig. 2. A projection of the whole structure along c is represented in Fig. 3, where one may note that: (a) cross linking of the cages forms large channels delimited by 12-membered rings and surrounded by 6 cages, and smaller ones delimited by distorted 8-membered rings between adjacent pairs of cages; (b) the exchangeable cations are distributed into three positions, (I) inside the cages, (II) in the channels between the cages, and (III) in the middle of the larger channels.

The free diameter of the large channels formed by 12-rings of tetrahedra is 7.4 Å assuming the effective radius of oxygen to be 1.35 Å. Channels of the same order of magnitude are rather rare in zeolites, being present only in faujasite, gmelinite, mordenite and offretite.

The analysis of the anisotropic temperature factors (Table 3) revealed small deviation from isotropy for all atoms, the maximum anisotropy occurring in the thermal parameters of (K, Na, Ca) in site II.

The mean T-O distances for mazzite are consistent with Si, Al disorder (Table 4).

The topological difference between this structure and that proposed by BARRER and VILLIGER (1969) for zeolite  $\Omega$  lies in the interconnection of the columns of cages, and it is a result of the different space group, P6<sub>3</sub>/mmc assumed from single crystal data for mazzite, compared to P6/mmm assumed from powder data for phase  $\Omega$ . The difference between the two is revealed by the absence of diffractions of the type hh2hl with l = odd in P6<sub>3</sub>/mmc. The same diffraction however are missing also in the powder data of phase  $\Omega$  (AIELLO and BARRER, 1970). Hence the two zeolites could have the same space group and the same framework.



Fig. 3. — The structure of mazzite projected along c. TO<sub>4</sub> tetrahedra pointing up are easily recognizable whereas those pointing down are shown only as triangles. Those with an edge normal to the projection plane can be distinguished because they form hexagonal rings around Mg. The positions and coordinations of the exchangeable cations may be better understood by comparing this Figure with Figs. 4, 5 and 6. Broken circles represent the dimensions of oxygens atoms, and indicate the free aperture of the main channels.

One of the characteristic features of mazzite as a zeolite is its high Mg-content. Mg<sup>++</sup>-ions occur in site I at the center of all the «gmelinite-type» cages (Fig. 4). Above and below each Mg<sup>++</sup>-ion has two H<sub>2</sub>O(2) molecules (100 % occupancy) and nine positions for water molecules [H<sub>2</sub>O(3) and H<sub>2</sub>O(4)] surround the Mg<sup>++</sup>-ion at its own level, but only four out of these nine positions can be occupied at the same time; as for instance, those joined to Mg<sup>++</sup> by a dashed line in Fig. 4. The TABLE 3

Observed and calculated structure factors (X 10). Unobserved reflections are marked with an asterisk

	 ~ • • •	. 10 PC	• K L	PO PC	H K L	PO FC	N K L 90 PC	
zer				37435599777584351259737411222233129393756755912112597255979557324557557557557557557557557557557557557557		######################################		

same figure shows also the positions of the framework oxygens relative to the  $Mg^{++}$ -water complex. In the dehydrated form Mg bonds to the three 0(1)'s of these rings and to one residual water molecule (RINALDI et al., 1975).

Occupancy of  $H_2O(3)$  and  $H_2O(4)$  must not be higher than 4/9 = 0.44, and the multiplicity factor was fixed at this value in the last cycles of the refinement, as said above. Essentially the Mg<sup>++</sup>-ions are octahedrally coordinated.

Further studies on the crystallization kinetics of zeolites containing the same building units as mazzite may well lead to the conclusion that the Mg-water complex acts as a template to the formation of «gmelinite-type cages». The same role would be played by the large organic TMA-ions in the crystallization of zeolite  $\Omega$ .



Fig. 4. — Coordination of water molecules around Mg in site 1 shown in projection along c. Three-digit numbers give the height over the projection plane as permillage of c.  $H_2O(2)$  is always present. Only four of the nine  $H_2O(3)$  and  $H_2O(4)$  molecules are present at the same time (for instance those joined to Mg with dashed lines). On the average, Mg coordinates octahedrally to 6 water molecules.

Site II is occupied about 50 % by a mixture of ions (in order of abundance:  $K \propto 42 \%$ , Na $\approx 5 \%$ , Ca $\approx 3 \%$  and empty 50 %). These cations (Fig. 5) coordinate mainly to framework-oxygens, two 0(2) and four 0(4), which form a rather distorted hexagon. The distances to 0(2) are slightly larger than those reported by SHANNON and PREWITT (1969) for 8-coordinated K<sup>+</sup>. The coordination is completed by two H<sub>2</sub>O(1) molecules, with an occupancy of 50 %; the overly short distances of these water molecules to the cations may be easily explained, as done in the legend of Fig. 5.

Fig. 6 is a detail of the content of the larger channels, with cation site III. Here the situation is complicated by many low occupancies, the higher ones being 89% for H<sub>2</sub>O(6) and 45\% for H<sub>2</sub>O(7), which determine the prevailing coordination pattern around Ca<sup>++</sup>; this can be described as follows: the Ca cations are

### TABLE 4

## Interatomic distances (Å) and angles (°) within the framework with e.s.d.'s on the last digit in parentheses

T(1)-0(1) T(1)-0(2) T(1)-0(4) Average 0(1)-0(2) 0(1)-0(4) 0(2)-0(4) 0(4)-0(4) T(2)-0(3) T(2)-0(4) T(2)-0(5) T(2)-0(6) Average 0(3)-0(4) 0(3)-0(5) 0(4)-0(5)	1.655(3) 1.641(2) 1.658(4)[x2] 1.653 2.685(5) 2.720(5)[x2] 2.674(4)[x2] 2.721(8) 1.642(2) 1.642(2) 1.645(2) 1.640(2) 1.640(2) 1.639 2.619(4) 2.699(5) 2.710(4) 2.708(5)	0(1)-T(1)-0(2)  0(1)-T(1)-0(4)  0(2)-T(1)-0(4)  0(4)-T(1)-0(4)  0(3)-T(2)-0(4)  0(3)-T(2)-0(5)  0(3)-T(2)-0(6)  0(4)-T(2)-0(6)  0(5)-T(2)-0(6)  T(1)-0(1)-T(1)  T(1)-0(2)-T(1)  T(1)-0(4)-T(2)  T(2)-0(3)-T(2)  T(2)-0(5)-T(2)  T(2)-0(6)-T(2)  T(2)-0(6) -T(2)  T(2)-0(6) -T(2) -T(2)  T(2)-0(6) -T(2) -T(2	109.1(4) $110.4(2)[x2]$ $108.3(2)[x2]$ $110.3(3)$ $106.4(2)$ $110.4(3)$ $111.3(2)$ $111.6(2)$ $110.5(2)$ $106.8(2)$ $149.2(5)$ $171.0(5)$ $144.6(2)$ $146.5(4)$ $138.0(3)$ $136.7(3)$
0(3) - 0(4) 0(3) - 0(5)	2.619(4) 2.699(5)	T(1)-O(4)-T(2) T(2)-O(3)-T(2)	144.6(2) 146.5(4)
0(3) - 0(6) 0(4) - 0(5) 0(4) - 0(6)	2.710(4) 2.708(5) 2.685(5)	T(2)-O(5)-T(2) T(2)-O(6)-T(2)	138.0(3) 136.7(3)
0(5)-0(6)	2.637(2)		

located on the c axis at z/c = 0.072 with an occupancy of 23 %. Six water positions occupied by H<sub>2</sub>O(6) and H<sub>2</sub>O(7) occur above and below the Ca site at the vertices of a hexagonal prism. More water molecules [H<sub>2</sub>O(5)] are located at approximately the same height as Ca and with an occupancy of 23 % in twelve positions of which only three can be occupied at the same time in accordance with statistical occupancy and possible distance restraints. The Ca position could actually be occupied by a random alternation of Ca and water molecules.

In short the walls of the wide channel are lined with water molecules, and the cations are set at regular intervals in the middle of these « water pipes ». This configuration is the most plausible, however the distribution of cations and water molecules in these wide channels is not as well defined as it may be in smaller cavities due to the considerable freedom of movement of the atomic species as evidenced by their high thermal motions.



Fig. 5. — Coordination of framework-oxygens and water molecules around the (K, Na, Ca) site II (occupancy factor = 50 %), shown in clinographic projection. The cation is at the center of a distorted hexagon with two 0(2) and four 0(4) at its corners. The distance from the lower cation to  $H_{2}O(1')$  (occupancy factor 50 %) is 1.63 Å, hence forbidden. The following assumption is proposed: when the upper cation position is empty and the lower is occupied, the two  $H_{2}O(1)$  are present and the two  $H_{2}O(1')$  are absent, and vice-versa.

An interestin relationship exists between the structures of mazzite and offretite (GARD and TAIT, 1972), which are associated at Mont Semiol. Both zeolites contain the «gmelinite-type» cages occupied by the hydrated Mg-ion, and in both of them the superimposition of these cages forms columns parallel to c. Offretite contains large channels surrounded by 12-rings of tetrahedra too, but the positions and the connections between the «gmelinite-type» cages are different; a rotation of 60° and translation of c/2 of the columns is necessary to trasform one structure into the other. Some similarities between the two could also be present in the distribution of the cations within the large channels.



Fig. 6. — Coordination of water molecules around Ca in site III shown here in projection along c. Three digit numbers give the heights over the plane of projection as permillage of c. Most abundant are  $H_2O(6)$  and  $H_2O(7)$  placed at z/c = 1/4 and -1/4, hence giving a hexagonal prism configuration around Ca, which lies nearly at z/c = 0.

#### Acknowledgements

Thanks are due to G. Gottardi for encouraging this research; to J. V. Smith and R. Rinaldi for useful discussion and the critical reading of the manuscript; to the donors of the Petroleum Research Fund administered by the American Chemical Society for grant-in-aid 6276 AC2 to J. V. Smith, which made the X-ray intensity data collection possible; and W. Lugli for the drawings.

The financial support of the Consiglio Nazionale delle Ricerche, Roma, is also acknowledged.

Cations, oxygens and water molecules: distances less than 3.40 Å, with e.s.d.'s on the last digit in parentheses

$K_Na_Ca=0(2)$	3.06(1)[x2]	$H_0(3) - 0(3)$	3.04(2)
$K_N a_C a_0(\Lambda)$	2.89(1) [x4]	$H^{2}_{0}(3^{1})-H_{0}(4^{1})$	1.37(2)*
$K_{Na}$ $Ca = U(4)$	2 80(1)[x2]	$H^{2}O(3^{+}) - H^{2}O(4^{+})$	2.63(2)
$X_{Na}(a-n 0(1))$	$\frac{1}{1} \frac{62}{1} \frac{1}{1} 1$	$\frac{1}{2}$ (0) $\frac{1}{2}$ (1)	
$\frac{1}{2}$	$1.03(1)[x_2]$	$H_{0}(A) = O(3)$	2,95(2)
	0.02(1)[~2]	$H^{2}O(4) = O(3)$	3,29(1)
$^{1}g-H_{2}(2)$	$2.03(1)[x_2]$	$H^{2}O(4^{+}) - H^{-}O(4^{+})$	$1.46(3)^*$
$^{\rm Mg-H}_{2}$ (3)	1.99(2)[x3]	$H^{2}_{2}(4^{\parallel}) = H^{2}_{2}(4^{\parallel})$	264(3)
$^{Mg-H^{-}O(4)}$	2.08(2) xo	$\frac{1}{2}$	2.04(3)
Ca_Ca	1 10(12)*	$H_{0}(5) = 0(5)$	2.93(3)
	$2 72(12)^*$	$H^{2}O(5) = O(6)$	2.62(2)
	$2 \cdot / 2 (13)$	$H^{2}O(5^{+}) - HO(5^{+})$	1.70(5)*
$2^{2}$	$2 \cdot 52(2) [x0]$	$H^{2}O(5^{1}) - H^{2}O(5^{11})$	3.36(7)
$a - H 0(5^{\circ})$	2.02(3)[x0]	$\mu^{2}O(51) - \mu^{2}O(5^{ V })$	2.55(3)
$2a - H_0(6')$	3.11(4)[x3]	$H^{2}O(51) - H^{2}O(5^{\vee})$	$1.00(5)^{*}$
$2^{2a-H_{2}}(7^{\prime\prime})$	$2.78(4) \lfloor x3 \rfloor$	$H^{2}O(51) - H^{2}O(5^{V})$	3, 23(5)
	<i>.</i>	$H^{2}O(5^{-1}) H^{2}O(6^{-1})$	1.03(3)*
$H_{2}^{0(1)-0(3)}$	3.21(1)	$H^{2}_{0}(5) = H^{2}_{0}(6)$	$1 \cdot 93(3)$
$H_{2}^{-0}(1) = 0(4)$	2.93(1)	$H_0(5) = H_0(0^{-1})$	2.03(3)
$H_{2}^{0}(1) - H_{2}^{0}(1)$	3.25(3)	$H_0(5^{-1}) - H_0(7^{-1})$	$2 \cdot 3 \cdot (3)$
$H_{2}^{*}0(1) - H_{2}^{*}0(1^{1})$	1.36(3)*	$H_2^{-0}(5^{-1}) - H_2^{-0}(7^{-1})$	2.30(3)
$H_{2}^{2}O(1) - H_{2}^{2}O(4)$	2.51(2)	-	a (a)
2 2		$H_{0}(6) - 0(5)$	3.03(2)
$H_0(2) = O(1)$	2.97(1)	$H_{2}^{0}(6') - H_{2}^{0}(7'')$	2.03(2)
$H_{0}^{2}(2) - H_{0}(3)$	2.84(2)	2 -	( . )
	0.01(1)	$H_0(7) = O(5)$	3.31(3)

The superscripts do not follow any specific rule, but are used solely to locate the corresponding atoms in Figs. 4. 5 and 6.

An asterisk indicates distances too short for simultaneous occupation of both sites.

The multiplicator of the interatomic distances related by symmetry is given in square brackets for cation polyhedra only.

### REFERENCES

- AIELLO R. and BARRER R. M. (1970) Hydrothermal chemistry of silicates. Part XIV. Zeolite crystallization in presence of mixed bases. J. Chem. Soc. (A), 1970, 1470-1475.
- BARRER R. M. and VILLIGER H. (1969) Probable structure of zeolite Ω. Chemm. Comm., 1969, 659-660.
- BUSING W.R., MARTIN K.O. and LEVY H.A. (1962) ORFLS, a Fortran crystallographic leastsquares refinement program. U. S. Nat. Tech. Infor. Serv., ORNL-TM-305.

CROMER D.T. and MANN J.B. (1968) - X-ray scattering factors computed from numerical Hartree-Fock wave functions. Acta Cryst., A24, 321-324.

GALLI E. (1974) - Mazzite, a zeolite. Cryst. Struct. Comm., 3, 339-344.

- GALLI E., PASSAGLIA E., PONGILUPPI D. and RINALDI R. (1974) Mazzite a new mineral, the natural counterpart of the synthetic zeolite  $\Omega$ . Contr. Mineral. and Petrol., 45, 99-105.
- GARD J. A. and TAIT J. M. (1972) The crystal structure of the zeolite offretite, K<sub>1.1</sub>Ca<sub>1.1</sub>Mg<sub>0.7</sub> [Si<sub>12.0</sub>Al<sub>2.2</sub>O<sub>30</sub>] • 15.2H<sub>2</sub>O. Acta Cryst., B28, 825-834.
- RINALDI R., PLUTH J.J. and SMITH J.V. (1975) Crystal structure of mazzite dehydrated at 600° C. Acta Cryst., B31, 1603-1608.
- SHANNON R. D. and PREWITT C. T. (1969) Effective ionic radii in oxides and fluorides. Acta Cryst., B25, 925-946.

UNION CARBIDE Co., Dutch Pat. 6,718,729 3rd August, 1967.