

The Crystal Structure of the Zeolite Ferrierite

BY PHILIP A. VAUGHAN

School of Chemistry, Rutgers, The State University, New Brunswick, N.J., U.S.A.

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A sample of the zeolite mineral ferrierite was found to have unit-cell dimensions $a=19.16$, $b=14.13$, $c=7.49$ Å (unit-cell content approximately $\text{Na}_{1.5}\text{Mg}_2\text{Si}_{30.5}\text{Al}_{5.5}\text{O}_{72} \cdot 18\text{H}_2\text{O}$) and to belong to space group *Immm*. The crystal structure was determined from three-dimensional X-ray data. Channels, whose size is defined by a ring of ten tetrahedra, exist parallel to the c axis in the aluminosilicate framework. Another prominent feature is the existence of large cavities which contain $\text{Mg}(\text{H}_2\text{O})_6^{2+}$ ions. Structurally, ferrierite most closely resembles mordenite and dachiardite. There is no evidence for ordering of metal atoms in the metal positions. It was not possible to locate the Na^+ ions or six of the eighteen water molecules.

Introduction

Ferrierite is a zeolite mineral which occurs near Kamloops Lake, British Columbia. A crystallographic description has been given by Staples (1955), who reported a unit-cell content represented approximately by $(\text{Na}, \text{K})_4\text{Mg}_2(\text{Si}_{30}\text{Al}_6)\text{O}_{72}(\text{OH})_2 \cdot 18\text{H}_2\text{O}$.

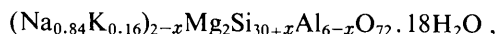
Experimental

Dr L. B. Sand of the Norton Company kindly supplied me with some crystals of ferrierite which he had collected at Kamloops Lake. The parameters of the orthorhombic unit cell were computed from measurements on zero-layer Weissenberg photographs which were also exposed to the sodium chloride powder pattern for calibration. The results are

$$\begin{aligned} a &= 19.156 \pm 0.005 \text{ \AA} \\ b &= 14.127 \pm 0.003 \\ c &= 7.489 \pm 0.003 \end{aligned}$$

Systematic absences indicate that the space group is *Immm*, *Imm2*, or *I222*. The density at room temperature, measured by the flotation method, is 2.136 g.cm^{-3} .

A chemical analysis of ferrierite was performed by R. M. Rebert of the Norton Company. The results, when combined with the above crystallographic data, indicate a unit-cell content which can be represented with good accuracy by



with $x=0.15$ computed from the Si:Al ratio, or 0.5 computed from the alkali content. The computed density is 2.11 g.cm^{-3} .

Our crystallographic results are in satisfactory agreement with those of Staples (1955), although he gives a rounded-off formula, based on Graham's (1918) analysis, of $(\text{Na}, \text{K})_4\text{Mg}_2\text{Si}_{30}\text{Al}_6\text{O}_{72}(\text{OH})_2 \cdot 18\text{H}_2\text{O}$, which indicates a higher alkali content.

Three-dimensional intensity data were obtained from three-film Weissenberg exposures of the $(hk0)$, $(hk1)$, $(hk2)$, $(hk3)$, $(hk4)$, $(hk5)$, $(hk6)$, $(0kl)$, $(1kl)$, $(2kl)$, and $(h0l)$ layer lines; and the corresponding $|F|_o$ values were placed on a common scale by a least-squares method of correlating reflections common to two or more sets of films. A total of 1131 reciprocal-lattice points were examined, and 674 measurable $|F|_o$ values were obtained, the remainder being unobserved on any of the films. Since it is essential that the unobserved data be included in the statistical procedures used in the structure determination, each unobserved intensity was recorded as $\frac{1}{3}I_m$, in which I_m is the estimated minimum observable intensity. This is the mean intensity under the assumption of a uniform distribution of F between $-|F|_m$ and $|F|_m$ (Hamilton, 1955). After correction for Lorentz and polarization factors, $|F|_o$ for each unobserved reflection was taken to be the smallest of the values of $3^{-1}|F|_m$ recorded for that reflection.

Structure determination

The approximate scale and over-all temperature factors were found by the method of Wilson (1942). In making the computation, the structure factors with any zero indices were omitted because the existence of mirror planes and twofold axes would make the mean values of the intensities of these special reflections larger by a factor of 2 (one zero index) or 4 (two zero indices) than those of the general reflections (Wilson, 1950). The normalized structure factors $|E|$ were then computed by the relation* (Hauptman & Karle, 1953):

$$E_{\mathbf{H}} = \sum_{j=1}^N g_j \exp(2\pi\mathbf{H} \cdot \mathbf{r}_j) = F_{\mathbf{H}} \exp[B(\sin \theta/\lambda)^2] / \left(\sum_{j=1}^N f_j^2 \right)^{\frac{1}{2}}, \quad (1)$$

in which

$$g_j = f_j / \left(\sum_{j=1}^N f_j^2 \right)^{\frac{1}{2}}.$$

The next task was to determine the probable space group. The mean value $\langle(E^2-1)^2\rangle^{\ddagger}$ should be approximately 2^{\ddagger} for centrosymmetric, and 1 for noncentrosymmetric structures. In this case, $\langle(E_{hkl}^2-1)^2\rangle^{\ddagger}$ was found to be 1.36 (reflections with a zero index omitted), which favors a centrosymmetric space group. Additional evidence can be obtained from the special planes or lines in the reciprocal lattice in which one or more index is zero. The results are summarized in Table 1. The theoretical values are those for the case of no atoms in special positions, and terms of order $N^{-\ddagger}$ (N =atoms per lattice point) have been neglected. From these results, the space group *Immm* was assumed, and at no time during the structure determination or refinement was there an experimental indication of lower symmetry. However, as will be mentioned in the discussion, a feature of the structure suggests the possibility of lower symmetry.

A trial structure was obtained by direct sign determination of a group of large structure factors. Regression formulas (Vaughan, 1959) used are

$$E_{h00} \approx \Sigma = c_1 S_{\frac{1}{2}h} + c_2 \sum_{k_1} T_{k_1} P_{\frac{1}{2}h, k_1} + c_3 \sum_{l_1} U_{l_1} Q_{\frac{1}{2}h, l_1}, \quad (2)$$

$$E_{h00} \approx \Sigma' = c'_1 \sum_{h_1 k_1} S_{h_1} T_{k_1} P_{\frac{1}{2}h-h_1, k_1} + c'_2 \sum_{h_1 l_1} S_{h_1} U_{l_1} Q_{\frac{1}{2}h-h_1, l_1}, \quad (3)$$

$$E_{hk0} \approx \Sigma'' = c''_1 \sum_{h_1 k_1} S_{h_1} T_{k_1} P_{\frac{1}{2}h-h_1, \frac{1}{2}k-k_1}, \quad (4)$$

in which

$$S_h = \sum_{k,l} (E_{hkl}^2/2^z - 1),$$

$$T_k = \sum_{h,l} (E_{hkl}^2/2^z - 1),$$

$$U_l = \sum_{h,k} (E_{hkl}^2/2^z - 1),$$

$$P_{hk} = \sum_l (E_{hkl}^2/2^z - 1),$$

$$Q_{hl} = \sum_k (E_{hkl}^2/2^z - 1),$$

and z = number of zero indices (0, 1, or 2) in hkl . Similar equations were used to determine signs of $0k0$,

* In this work, the structure factor will be referred to a single lattice point instead of to a unit cell. Note also that E_H does not have a mean-square value of unity for all classes of reflections.

$00l$, $h0l$, and $0kl$ structure factors. The coefficients c in the above equations are obtained by solving the set of variance-covariance equations. If the individual summations on the right sides of (2), (3), and (4) are labeled $T_1, T_2, T_3, T'_1, T'_2$, and T''_1 , we have, approximately,

$$\begin{aligned} \overline{E_{h00} T_1} &= 4n_1 S_3, \\ \overline{E_{h00} T_2} &= 16n_2 S_5, \\ \overline{E_{h00} T_3} &= 16n_3 S_5, \\ \overline{E_{h00} T'_1} &= 64n'_1 S_7, \\ \overline{E_{h00} T'_2} &= 64n'_2 S_7, \\ \overline{E_{hk0} T''_1} &= 32n''_1 S_7, \\ \overline{T_1^2} &= 2n_1(1 + n_1 S_4), \\ \overline{T_2^2} &= 4n_2(1 + 16n_2 S_8), \\ \overline{T_3^2} &= 4n_3(1 + 16n_3 S_8), \\ T_1 \overline{T_2} &= 16n_1 n_2 S_6, \\ \overline{T_1 T_3} &= 16n_1 n_3 S_6, \\ \overline{T_2 T_3} &= 64n_2 n_3 S_6, \\ (\overline{T'_1})^2 &= 8n'_1(1 + 128n'_1 S_{12}), \\ (\overline{T'_2})^2 &= 8n'_2(1 + 128n'_2 S_{12}), \\ \overline{T'_1 T'_2} &= 1024n'_1 n'_2 S_{12}, \\ (\overline{T''_1})^2 &= 8n''_1(1 + 64n''_1 S_{12}), \end{aligned} \quad (5)$$

in which n_i is the total number of terms in the corresponding summation, and $S_n = \sum_{j=1}^N g_j^n$. In the above equations, terms of higher order (higher subscripts on S_n) have been neglected. It is evident that equations (2) and (3) could be combined to give a single five-term formula, but this was not done in this case.

The above equations were applied to all of the $h00$, $0k0$, and $00l$ reflections, and to all of the $hk0$, $h0l$, and $0kl$ reflections with E magnitudes greater than 1.5. Since the probability that E and Σ have the same sign is approximated by

$$P_+ = \frac{1}{2} + \frac{1}{2} \tanh(|E\Sigma|/\sigma^2), \quad (6)$$

the quantity $|E\Sigma|/\sigma^2$ is a measure of the probability of a correct sign determination. In 31 cases this quan-

Table 1. Symmetry tests with normalized structure factors

	Theoretical for <i>Immm</i>		Experimental		Number of terms
	$\langle E^2 - 1 \rangle$	$\langle (E^2 - 1)^2 \rangle^{\ddagger}$	$\langle E^2 - 1 \rangle$	$\langle (E^2 - 1)^2 \rangle^{\ddagger}$	
<i>hkl</i>	0.0	1.4	0.02	1.36	809
<i>hk0</i>	1.0	3.0	1.15	2.67	160
<i>h0l</i>	1.0	3.0	0.75	2.39	76
<i>0kl</i>	1.0	3.0	1.37	3.66	62
<i>h00</i>	3.0	6.4	1.56	3.08	12
<i>0k0</i>	3.0	6.4	6.89	11.60	8
<i>00l</i>	3.0	6.4	10.50	16.09	4

tity was greater than 2.0, and these were used with the probable relation $S_H = S_K S_{H-K}$ to test the internal consistency of the set and to determine more signs. Three of the initial set of 31 signs were found to be wrong. Among the signs determined with relatively high probability by this procedure were 40 $hk0$ reflections with large structure factors. As a first attempt at obtaining a trial structure, these were used to calculate an electron density projection along z . It was found that the aluminosilicate framework ($M_{36}O_{72}$) structure could be deduced from this projection. Although the projection was considerably distorted owing to omission of terms, all of the 40 signs eventually proved to be correct.

To refine the structure, two more successive electron density projections along z were computed, and the

last of these was used, with the known geometry of the tetrahedral linkages involved, to compute the z coordinates of the metal and oxygen atoms. A three-dimensional electron-density map was then computed. At this point, a large peak was observed at the origin of the unit cell, which was surrounded by a pair of peaks along the z axis and eight smaller (equivalent to one-half an O atom) peaks in the $x-y$ plane. This group of peaks was interpreted as a disordered $Mg(H_2O)_6^{2+}$ ion. The ion has two possible configurations, which differ by a rotation of 42° about the z axis. Since these configurations are related by mirror planes which are part of the crystallographic symmetry, each position occurs 50% of the time.

Refinement was carried out by computing two more three-dimensional electron-density maps, and then

Table 2. Atomic coordinates and their standard deviations

M = Si, Al				
Atom	Point symmetry	x	y	z
4 M(1)	mm	0.1548 (4)	0	0
8 M(2)	m	0.0841 (3)	0.2024 (4)	0
8 M(3)	m	0.2727 (3)	0	0.2905 (8)
16 M(4)	1	0.3232 (2)	0.2019 (3)	0.2067 (5)
4 O(1)	mm	0	0.2131 (18)	0
4 O(2)	mm	0.2528 (15)	0	$\frac{1}{2}$
8 O(3)	m	0.1025 (10)	0.0882 (12)	0
8 O(4)	m	0.2039 (10)	0	0.1776 (23)
8 O(5)	i	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
8 O(6)	m	0.1610 (10)	0.2833 (12)	$\frac{1}{2}$
16 O(7)	1	0.1155 (7)	0.2497 (7)	0.1796 (15)
16 O(8)	1	0.3202 (6)	0.0907 (7)	0.2459 (16)
4 O(9)	mm	0	0	0.2389 (32)
4 O(10)*	m	0.0912 (24)	0.0691 (39)	$\frac{1}{2}$
4 O(11)*	m	0.0347 (27)	0.1403 (29)	$\frac{1}{2}$
2 Mg	mmm	0	0	$\frac{1}{2}$
0.92 Na†	mm	0.4285 (24)	0	0

* One-half O in an eightfold position.

† Or oxygen.

Table 3. Thermal parameters $U_{ij} \times 10^3$ in the expression $\exp[-2\pi^2(U_{11}h^2b_1^2 + U_{22}k^2b_2^2 + U_{33}l^2b_3^2 + 2U_{12}hkb_1b_2 + 2U_{13}hkb_1b_3 + 2U_{23}klb_2b_3)]$, and their standard deviations

M = Si, Al						
Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
M(1)	30 (4)	19 (3)	17 (4)			
M(2)	24 (2)	23 (2)	12 (2)	2 (2)		
M(3)	31 (3)	19 (2)	26 (3)		-4 (2)	
M(4)	33 (2)	20 (1)	26 (2)	0 (2)	-1 (2)	-4 (2)
O(1)	43 (13)	57 (16)	46 (15)			
O(2)	100 (20)	18 (10)	25 (12)			
O(3)	66 (13)	34 (9)	114 (18)	16		
O(4)	59 (11)	119 (17)	20 (9)		-13 (9)	
O(5)	78 (12)	43 (9)	50 (11)	6 (9)	-5 (10)	0 (9)
O(6)	83 (13)	48 (10)	14 (8)	10 (9)		
O(7)	61 (8)	67 (8)	40 (7)	-7 (7)	-3 (7)	-21 (7)
O(8)	59 (7)	26 (5)	59 (8)	4 (5)	3 (7)	4 (5)
O(9)	53 (14)	48 (13)	38 (14)			
O(10)	101 (33)	175 (48)	10 (18)	-51 (33)		
O(11)	142 (49)	52 (25)	156 (49)	-56 (27)		
Mg	24 (7)	48 (10)	53 (9)			
Na	18 (28)	81 (46)	15 (30)			

subjecting the resulting coordinates to six cycles of block-diagonal least squares. The atoms included in this refinement procedure were $Mg_2O_{12}M_{36}O_{72}$ per unit cell, and f_{Si} was used for the scattering factors of all the framework metal atoms because there was no evidence of any significant ordering of the Al and Si atoms. All thermal parameters were included, and the final R value was 0.118.

Since there were six water molecules and one to two Na^+ ions per unit cell not yet accounted for, a Fourier difference map was computed in an attempt to locate some of these atoms. Examination of the channel regions in this difference map revealed only one peak which would in any reasonable way be distinguished from the 'error background', and this peak was only as high as about 0.3 of an O atom. There were several other positive regions, but these were very irregular and had maxima only about 10–15% as high as the O atoms on an ordinary Fourier synthesis. Since there were also negative regions of the same order of magnitude, no attempt was made to locate any more atoms.

Although the additional peak could be due to O, Na, or some combination of these, f_{Na} was assigned to it and the parameters were subjected to seven more cycles of block-diagonal least-squares refinement. The occupancy factor of the latter position was included as a parameter in this refinement, and the final value for this quantity was 0.23 ± 0.05 . Thus, we have accounted for only one of the missing atoms. We conclude that the remaining atoms have no discernible crystallographic periodicity, except, of course, that they must be located within the open channels in the structure. The final R value was 0.107. The final positional and thermal parameters are given in Tables 2 and 3, and the final observed and calculated structure factors are listed in Table 5.

Discussion

A projection of the structure along [001] is given in Fig. 1, and the linkages of the MO_4 tetrahedra in the $M_{36}O_{72}$ framework are illustrated in Fig. 2. One notes the large number of five-membered rings and smaller numbers of six-, eight-, and ten-membered rings of tetrahedra. An interesting feature of the structure is the existence of channels parallel to the c axis and centered at $x = \frac{1}{2}, y = 0$, and $x = 0, y = \frac{1}{2}$. These channels are roughly elliptical in cross section, have major and minor diameters of 5.4 and 4.2 Å (van der Waals radius of oxygen assumed to be 1.4 Å), and cross-sectional areas of about 18 Å². They are clearly responsible for the characteristic zeolite properties of ferrierite and most likely contain water and sodium ions. However, as mentioned above, the atoms in the channels are highly disordered.

The aluminosilicate structure also contains large cavities centered at $0, 0, \frac{1}{2}$ and $\frac{1}{2}, \frac{1}{2}, 0$. These cavities are roughly spherical with diameters of about 7 Å. They are connected to the large channels by 'windows', defined by eight MO_4 tetrahedra and perpendicular to

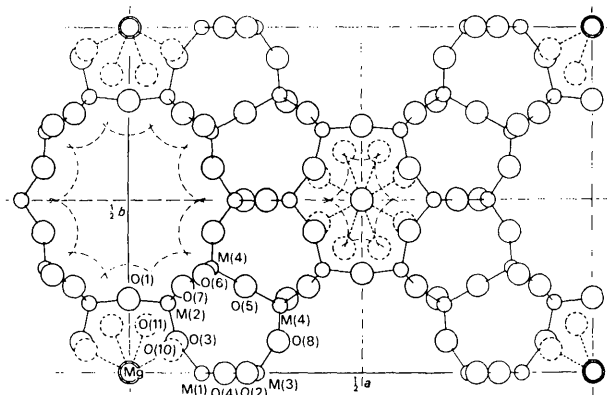


Fig. 1. Projection of the structure of ferrierite along the z axis. The dotted lines give the two orientations of $Mg(H_2O)_6^{2+}$. Atom O(9) coincides with Mg at the origin and at $\frac{1}{2}, \frac{1}{2}$ in this projection. The dashed arcs indicate van der Waals radii for oxygen.

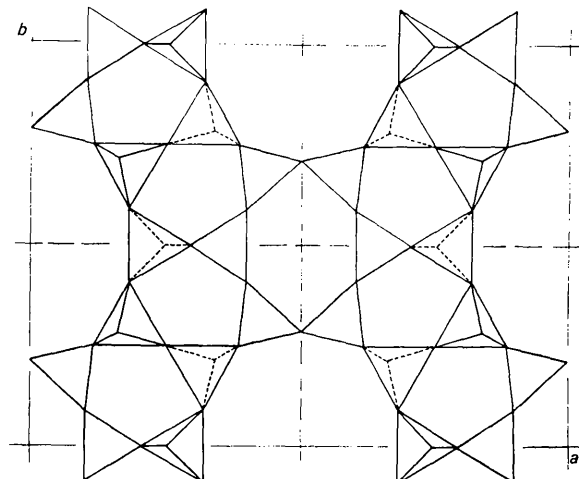


Fig. 2. Projection of the aluminosilicate framework in ferrierite along the z axis.

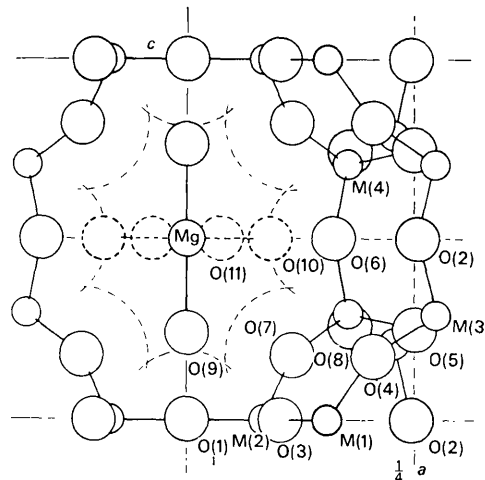


Fig. 3. Projection of the structure of ferrierite along the y axis.

the *b* axis, which have diameters of 4.7 and 3.4 Å, and cross-sectional areas of 12 Å². These 'windows' can be seen in Fig. 3, which is a projection of the structure onto the *x,z* plane. The cavities contain Mg(H₂O)₆²⁺ ions, which are disordered as described above. A view of one of these cavities, with the two equivalent positions of the Mg(H₂O)₆²⁺ ion, is shown in Fig. 4. It is interesting to note that prolonged leaching with hot acid does not remove a significant amount of Mg²⁺ from ferrierite.* It appears from the structure of the cavities that four water molecules would have to be stripped from this ion in order to allow it to pass through a 'window' into a large channel. This is evidently a very slow process at moderate temperatures. It is also possible that the diffusion of (partially) hydrated Mg²⁺ ions in the channels occurs rather slowly.

A list of important distances and angles in ferrierite is given in Table 4. It is clear that the distribution of Al and Si on the metal sites is essentially random, although M(2) might be somewhat richer in Al than the other sites. In general, the M–O distances are low compared with expectations based on the analysis of Smith & Bailey (1963). According to their graph† for framework aluminosilicates, the average M–O distance for an aluminum content of 15% should be 1.631 Å. The actual value in ferrierite is 1.605 Å. It is possible that tetrahedral M–O distances are somewhat shorter in zeolites than in the more compact feldspar structures which Smith & Bailey used in the construction of their graph. One notes that the average reported M–O distances in mordenite (Meier, 1961) and dachiardite (Gottardi & Meier, 1963) are 1.602 and 1.625 Å respectively, while the values based on the graph are 1.633 and 1.640 Å.

* Private communication from Dr L. B. Sand of the Norton Company.

† The graph is represented analytically by the expression $d = 1.610 + 0.14X$, in which *X* is the atom fraction of aluminum in the metal sites.

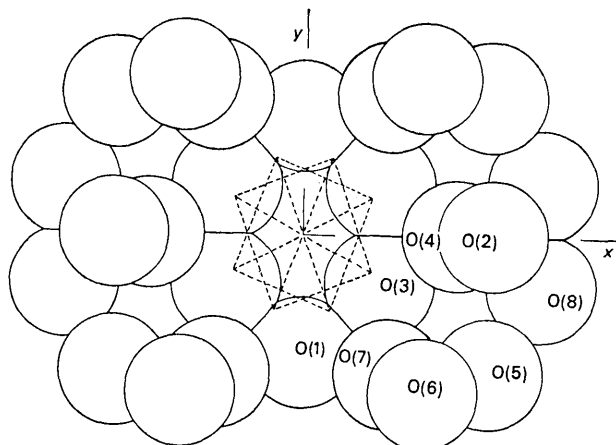


Fig. 4. View of the cavities in the aluminosilicate framework in ferrierite. The circles represent the van der Waals radii (1.4 Å) of the framework oxygen atoms, and the Mg(H₂O)₆²⁺ octahedron is shown by dotted lines in its two orientations.

Table 4. Bond lengths and angles in ferrierite

(a) M–O bond lengths	
2M(1)–O(3)	1.589 Å
2M(1)–O(4)	1.629
1M(2)–O(1)	1.619
1M(2)–O(3)	1.651
2M(2)–O(7)	1.618
1M(3)–O(2)	1.615
1M(3)–O(4)	1.567
2M(3)–O(8)	1.606
1M(4)–O(5)	1.592
1M(4)–O(6)	1.591
1M(4)–O(7)	1.603
1M(4)–O(8)	1.599

Over-all average M–O distance: 1.605 Å
 Approximate standard deviation for M–O bonds: 0.013 Å

(b) O–M–O bond angles	
1O(3)–M(1)–O(3)	102.5°
4O(3)–M(1)–O(4)	111.2
1O(4)–M(1)–O(4)	109.5
1O(1)–M(2)–O(3)	107.7
2O(1)–M(2)–O(7)	109.3
2O(3)–M(2)–O(7)	108.9
1O(7)–M(2)–O(7)	112.5
1O(2)–M(3)–O(4)	109.0
2O(2)–M(3)–O(8)	109.6
2O(4)–M(3)–O(8)	111.4
1O(8)–M(3)–O(8)	105.8
1O(5)–M(4)–O(6)	108.0
1O(5)–M(4)–O(7)	110.8
1O(5)–M(4)–O(8)	110.5
1O(6)–M(4)–O(7)	108.8
1O(6)–M(4)–O(8)	108.3
1O(7)–M(4)–O(8)	110.4

Approximate standard deviation for O–M–O angles: 0.7°

(c) M–O–M angles	
M(2)–O(1)–M(2')	169.2°
M(3)–O(2)–M(3')	152.7
M(1)–O(3)–M(2)	153.6
M(1)–O(4)–M(3)	157.9
M(4)–O(5)–M(4')	180.0
M(4)–O(6)–M(4')	153.3
M(2)–O(7)–M(4)	152.9
M(4)–O(8)–M(3)	147.4

Approximate standard deviation for M–O–M angles: 0.9°

(d) Mg–O distances and angles	
2Mg–O(9)	1.956 Å
2Mg–O(10)	2.001
2Mg–O(11)	2.090
O(10)–Mg–O(11)*	100.7°

* Within one orientation of Mg(H₂O)₆²⁺

(e) Water–oxygen nearest (less than 3.75 Å) distances	
4O(9)–O(3)	2.934
2O(9)–O(1)	3.500
2O(3)–O(9)–O(3)†	104.9°
O(10)–O(2)	3.246
O(10)–O(6)	3.308
2O(10)–O(4)	3.383
2O(10)–O(7)	3.533
O(11)–O(6)	3.152
2O(11)–O(7)	3.247

† Atoms O(3) and O(3') related by a twofold axis.

graphic center of symmetry. It appears that it would be difficult to discover, at least from the present data, which, if either, of these situations exists. If the true symmetry were *Imm* or *I222*, one would expect the thermal ellipsoids (Table 3) to be, in most cases at least, prolate spheroids because of the splittings imposed by the extra symmetry. Although several of the atoms, notably O(2), O(3), and O(4), show appreciable elongation, the overall amount of anisotropy does not seem unusual and O(5) itself is not particularly distorted. There is also no significant directional trend. The r.m.s. displacements in the *x, y, z* directions are 0.26, 0.23, and 0.22 Å for framework O, and 0.17, 0.14, and 0.15 Å for framework M, respectively. In view of these negative inferences, no attempt was made to find a structure of lower symmetry. The possibility of random, essentially static, displacements of O(5) (accompanied, perhaps, by concerted displacements of the neighboring M(4) atoms) cannot be excluded. A displacement of 0.2 Å from the M-M line would produce an angle of 166°. Such a disorder would be essentially indistinguishable from ordinary thermal motion.

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The Crystal and Molecular Structure of Aminomalonic Acid

BY J. A. KANTERS, J. KROON, P. T. BEURSKENS* AND J. A. VLIEGENTHART†

Laboratorium voor Kristalchemie, Rijksuniversiteit, Utrecht, The Netherlands

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Crystals of aminomalonic acid are orthorhombic ($P2_1cn$) with $a=4.990$, $b=8.507$ and $c=10.854$ Å ($Z=4$). The structure was solved in projection by direct methods applying three-dimensional structure factors, and refined with 560 diffractometer data to a final R value of 0.029. As both enantiomers of the zwitterionic molecule are present in the structure, the crystals are racemic despite the non-centrosymmetry of the space group. A rigid three-dimensional network is formed by extensive hydrogen bonding.

Introduction

From investigations (e.g. Marsh, 1958; Itaka, 1960, 1961; Pasternak, 1956) evidence has been adduced that amino acids and peptides are zwitterionic in the crystalline state. In aminodicarboxylic acids such as aspartic acid and glutamic acid the question arises which of the acid groups loses its proton. As far as we know, glutamic acid is the only aminodicarboxylic acid yet investigated (Hirokawa, 1955). In that analysis an indication of the configuration of the zwitterion was obtained from the dimensions of the carboxyl groups and from the two-dimensional difference Fourier syntheses.

In aminomalonic acid there are two equivalent carboxyl groups neighbouring the amino group, and this implies two possibilities: the molecule is non-zwitterionic ($\text{HOOC-CHNH}_2\text{-COOH}$) with two equivalent carboxyl groups, or zwitterionic ($\text{HOOC-CHNH}_3^+\text{-COO}^-$), in which case a molecule with an asymmetric carbon atom will result.

Experimental

Aminomalonic acid was synthesized from bromomalonic acid and ammonia. The literature mentions water of crystallization and melting points ranging from 109 to 136°C. Our crystals, which were obtained by slow evaporation of an aqueous solution at room temperature, did not contain water of crystallization and decomposed at 136°C.

* Present address: Laboratorium voor Anorganische Chemie, Catholic University, Nijmegen, The Netherlands.

† Permanent address: Laboratorium voor Organische Chemie, Rijksuniversiteit, Utrecht, The Netherlands.