

tive temperature factor' represents not only true thermal vibration but also some spread in position of the atom due to spatial disorder.

Table 3 lists isotropic B values determined in the course of the refinement procedure for the measurements on Schmirntal albite at 20, 300 and 600°C, and on Ramona albite at -180°C (Williams, 1961). When plotted against absolute temperature (Fig. 2) it is seen that for each kind of atom the B - T variation is very closely linear in the range -180 to 300°C, so that extrapolation to $T=0$ is justified. For sodium, aluminium and silicon atoms the extrapolation gives values of B very close to 0, whereas for oxygen atoms (at $T=0$) $B > 0$.

Table 3. *Low albite. Isotropic temperature factors B (Å²)*

	(WM, 1964) -180°C	(S ₂) 20°C	(S ₂) 300°C	(S ₂) 600°C
Na	1.0 (3)	3.2 (1)	5.6 (1)	6.7 (2)
Al	0.15 (6)	0.72 (6)	1.04 (9)	1.1 (1)
Si (average)	0.18 (6)	0.63 (4)	0.94 (6)	1.20 (8)
O (average)	0.38 (6)	1.01 (6)	1.65 (7)	2.0 (1)

Notes. Standard deviations are in brackets and refer to the last figure given.

Measurements on Schmirntal second fragment (S₂) and from Williams & Megaw (1964).

The difference between Na, Al and Si on the one hand, and O on the other, may be taken as evidence in support of a model in which the *position* of the Na atom is as clearly defined as are the positions of Al and Si atoms at the centres of their tetrahedral groups. Its large anisotropy is then due to anisotropic thermal vibration, not to positional disorder. By contrast, the O atoms show some positional disorder arising from the differences in Si-O and Al-O bond lengths and incomplete Al,Si order.

6. Conclusion

Measurements of diffraction intensities from low albite at 300 and 600°C have been used to study the anisotropy of the sodium atom as seen in [100] projection. Comparison with previous studies at room temperature and at -180°C provides strong support for the view that the observed anisotropy represents a true anisotropic thermal vibration of the sodium atom.

We are indebted to Mrs K. M. Hall for assistance with the interpretation of these measurements and to Mrs J. C. Matthewman for help with the computing, which was carried out on TITAN in the Mathematical Laboratory, Cambridge. This research forms part of a project supported by generous grants from D.S.I.R. and (more recently) N.E.R.C. One of us (S.Q.) is indebted to the Italian C.N.R. for the award of a N.A.T.O. Fellowship in 1964.

References

- FERGUSON, R. B., TRAILL, R. J. & TAYLOR, W. H. (1958). *Acta Cryst.* **11**, 331.
 FORSYTH, J. B. & WELLS, M. (1959). *Acta Cryst.* **12**, 412.
 QUARENI, S. (1969). *Z. Kristallogr.* **128**, 294.
 RIBBE, P. H., FERGUSON, R. B. & TAYLOR, W. H. (1962). *Norsk Geol. Tidsskr.* **42** (2), 152.
 RIBBE, P. H., FERGUSON, R. B., TRAILL, R. J. & TAYLOR, W. H. (1963). *Proc. Geol. Soc. Amer. Ann. Meetings*, New York, 136A.
 RIBBE, P. H., MEGAW, H. D. & TAYLOR, W. H. (1969). *Acta Cryst.* **B25**, 1503.
 TOKONAMI, M. (1965). *Acta Cryst.* **19**, 486.
 WILLIAMS, P. P. (1961). Ph. D. Thesis, Cambridge.
 WILLIAMS, P. P. & MEGAW, H. D. (1964). *Acta Cryst.* **17**, 882.

Acta Cryst. (1971). **B27**, 285

The Molecular and Crystal Structure of Hippuric Acid

BY HANS RINGERTZ

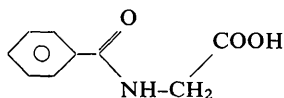
Department of Medical Physics, Karolinska Institutet and Department of Radiology, Karolinska Sjukhuset, S-10401 Stockholm, Sweden

(Received 26 February 1970)

Hippuric acid, C₆H₅.CO.NH.CH₂.COOH, crystallizes with four molecules in an orthorhombic unit cell with $a=8.874$, $b=10.577$, $c=9.117$ Å, space group $P2_12_12_1$. The structure has been determined by direct methods and refined by full-matrix least-squares computations. The final R value is 5.8%. The benzene ring, the peptide part and the carboxylic group are planar and twisted with respect to each other. The molecules are held together in three dimensions by one O-H...O and one N-H...O hydrogen bond to the peptide oxygen atom.

Introduction

Hippuric acid



is formed in mammals when benzoic acid is detoxicated by conjugation with glycine. It is excreted in urine and constitutes about a half per cent of the nitrogen excretion in man. The crystallographic and optical data of hippuric acid have been given by Ringertz (1969).

Experimental

Commercially available hippuric acid was recrystallized in water. The cell axes *a* and *b* were determined

from photographic measurements of high-angle reflexions with Cu *K*α radiation ($\lambda_{K\alpha 1} = 1.54051 \text{ \AA}$). The *c* axis was determined with a Philips automatic single-crystal diffractometer PAILRED using Mo *K*α radi-

Table 1. Final observed and calculated structure factors

The sign * represents a 'less than' reflexion. The columns are *l*, 10*F*_o, 10*F*_c, 10*A* and 10*B*.

<i>l</i>	10 <i>F</i> _o	10 <i>F</i> _c	10 <i>A</i>	10 <i>B</i>
0	0	0	0	0
1	100	100	100	100
2	200	200	200	200
3	300	300	300	300
4	400	400	400	400
5	500	500	500	500
6	600	600	600	600
7	700	700	700	700
8	800	800	800	800
9	900	900	900	900
10	1000	1000	1000	1000
11	1100	1100	1100	1100
12	1200	1200	1200	1200
13	1300	1300	1300	1300
14	1400	1400	1400	1400
15	1500	1500	1500	1500
16	1600	1600	1600	1600
17	1700	1700	1700	1700
18	1800	1800	1800	1800
19	1900	1900	1900	1900
20	2000	2000	2000	2000
21	2100	2100	2100	2100
22	2200	2200	2200	2200
23	2300	2300	2300	2300
24	2400	2400	2400	2400
25	2500	2500	2500	2500
26	2600	2600	2600	2600
27	2700	2700	2700	2700
28	2800	2800	2800	2800
29	2900	2900	2900	2900
30	3000	3000	3000	3000
31	3100	3100	3100	3100
32	3200	3200	3200	3200
33	3300	3300	3300	3300
34	3400	3400	3400	3400
35	3500	3500	3500	3500
36	3600	3600	3600	3600
37	3700	3700	3700	3700
38	3800	3800	3800	3800
39	3900	3900	3900	3900
40	4000	4000	4000	4000
41	4100	4100	4100	4100
42	4200	4200	4200	4200
43	4300	4300	4300	4300
44	4400	4400	4400	4400
45	4500	4500	4500	4500
46	4600	4600	4600	4600
47	4700	4700	4700	4700
48	4800	4800	4800	4800
49	4900	4900	4900	4900
50	5000	5000	5000	5000
51	5100	5100	5100	5100
52	5200	5200	5200	5200
53	5300	5300	5300	5300
54	5400	5400	5400	5400
55	5500	5500	5500	5500
56	5600	5600	5600	5600
57	5700	5700	5700	5700
58	5800	5800	5800	5800
59	5900	5900	5900	5900
60	6000	6000	6000	6000
61	6100	6100	6100	6100
62	6200	6200	6200	6200
63	6300	6300	6300	6300
64	6400	6400	6400	6400
65	6500	6500	6500	6500
66	6600	6600	6600	6600
67	6700	6700	6700	6700
68	6800	6800	6800	6800
69	6900	6900	6900	6900
70	7000	7000	7000	7000
71	7100	7100	7100	7100
72	7200	7200	7200	7200
73	7300	7300	7300	7300
74	7400	7400	7400	7400
75	7500	7500	7500	7500
76	7600	7600	7600	7600
77	7700	7700	7700	7700
78	7800	7800	7800	7800
79	7900	7900	7900	7900
80	8000	8000	8000	8000
81	8100	8100	8100	8100
82	8200	8200	8200	8200
83	8300	8300	8300	8300
84	8400	8400	8400	8400
85	8500	8500	8500	8500
86	8600	8600	8600	8600
87	8700	8700	8700	8700
88	8800	8800	8800	8800
89	8900	8900	8900	8900
90	9000	9000	9000	9000
91	9100	9100	9100	9100
92	9200	9200	9200	9200
93	9300	9300	9300	9300
94	9400	9400	9400	9400
95	9500	9500	9500	9500
96	9600	9600	9600	9600
97	9700	9700	9700	9700
98	9800	9800	9800	9800
99	9900	9900	9900	9900
100	10000	10000	10000	10000

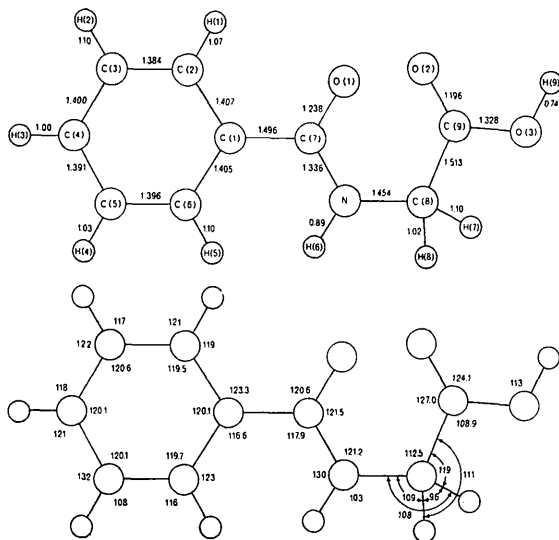


Fig. 1. Diagrams showing bond lengths and angles in the hippuric acid molecule.

tion. The following dimensions of the orthorhombic unit-cell were observed. The refractive indices refer to the crystallographic axes.

$$\begin{array}{ll}
 a = 8.874 \pm 2 \text{ \AA} & \beta = 1.592^\circ \\
 b = 10.577 \pm 3 & \gamma = 1.760 \\
 c = 9.117 \pm 3 & \alpha = 1.535
 \end{array}$$

Systematic absences were $h00$, $0k0$ and $00l$ with h , k and l respectively equal to $2n+1$, space group $P2_12_12_1$. $D_{\text{obs}} = 1.385 \text{ g.cm}^{-3}$ and $D_{\text{calc}} = 1.390 \text{ g.cm}^{-3}$, assuming $Z=4$. Two sets of reflexion data were recorded using two small crystals measuring approximately $0.15 \times 0.15 \times 0.15 \text{ mm}$. The first data set was collected using Ni-filtered $\text{Cu } K\alpha$ radiation and a General Electric single-crystal orienter which was operated manually. The second set of data was collected with a Philips automatic single-crystal diffractometer, PAIL-

RED, using monochromatized $\text{Mo } K\alpha$ radiation. In the first case 1098 structure amplitudes were obtained of which the 112 weakest were regarded as not observable. The two sets of data were corrected for Lorentz and polarization factors and put on an absolute scale. It was found that there was strong extinction of the most intense reflexions in the first data set and accordingly the 25 highest structure amplitudes were taken from the second data set. The E values were then calculated, giving the following statistical averages

	$\{E\}$	$\{E\}$	$\{ E^2-1 \}$
Observed	0.840	1.000	0.797
Theoretical for acentric	0.886	1.000	0.736
Theoretical for centric	0.798	1.000	0.968

Structure determination

The determination of the structure took four years and most crystallographic methods have been applied. However the optical indicatrix and the strength of the 102 and 202 reflexions indicated planar molecules with all parts parallel to the b axis and with the molecules inclined about 70° to each other. Spherical Patterson sections at 1.4 and 2.4 could be explained in detail by an essentially planar molecular model. In retrospect all assumptions were found to have been correct except that the carboxyl group was inclined at 85° with respect to the rest of the molecule and not coplanar with it.

The structure was finally solved using direct methods in a computer program series, *GAASA* 1-7 (Lindgren, Lindqvist & Nyborg, 1970). 273 reflexions with $E \geq 1.2$ were used in a symbolic addition procedure having a basic set of 10 symbols which were given to the strongest normalized structure factors taking part in the largest number of Sayre triplets. The number of symbols was then reduced on a statistical basis until 4 were left after 7 cycles:

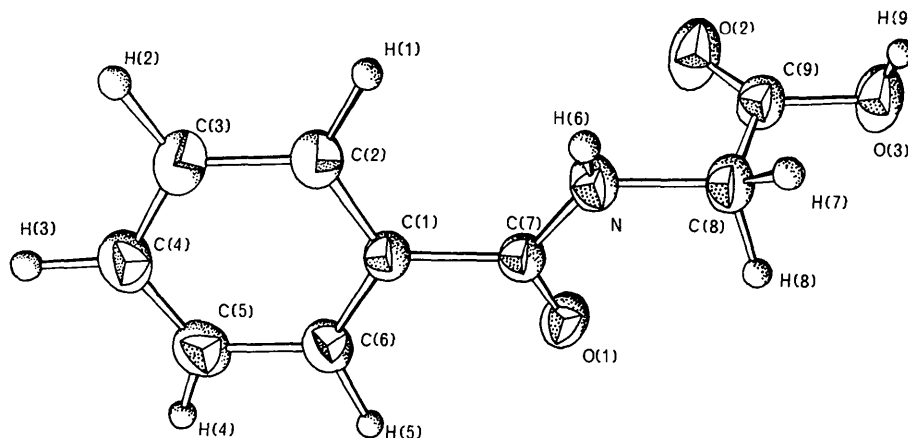


Fig. 2. Thermal ellipsoid representation of a hippuric acid molecule showing the labelling of the atoms. The ellipsoids enclose 50% probability. The hydrogen atoms are indicated by small spheres.

Table 3. Distances and angles of the hippuric acid molecule, with estimated standard deviations

Non-hydrogen intramolecular distances		Distances to hydrogen atoms	
C(1)–C(2)	1.407 (7) Å	C(2)–H(1)	1.07 (6) Å
C(1)–C(6)	1.405 (6)	C(3)–H(2)	1.10 (7)
C(1)–C(7)	1.496 (6)	C(4)–H(3)	1.00 (6)
C(2)–C(3)	1.384 (6)	C(5)–H(4)	1.03 (6)
C(3)–C(4)	1.400 (8)	C(6)–H(5)	1.10 (6)
C(4)–C(5)	1.391 (8)	N—H(6)	0.89 (6)
C(5)–C(6)	1.396 (7)	C(8)–H(7)	1.10 (6)
C(8)–C(9)	1.513 (7)	C(8)–H(8)	1.02 (6)
C(7)–N	1.336 (6)	O(3)–H(9)	0.74 (7)
C(8)–N	1.454 (6)		
C(7)–O(1)	1.238 (5)	Angles involving hydrogen atoms	
C(9)–O(2)	1.196 (6)	C(1)–C(2)–H(1)	119 (3)°
C(9)–O(3)	1.328 (5)	C(3)–C(2)–H(1)	121 (3)
Angles involving non-hydrogen atoms		C(2)–C(3)–H(2)	117 (3)
C(2)–C(1)–C(6)	120.1 (4)°	C(4)–C(3)–H(2)	122 (3)
C(2)–C(1)–C(7)	123.3 (4)	C(3)–C(4)–H(3)	118 (4)
C(6)–C(1)–C(7)	116.6 (4)	C(5)–C(4)–H(3)	121 (4)
C(1)–C(2)–C(3)	119.5 (5)	C(4)–C(5)–H(4)	132 (3)
C(2)–C(3)–C(4)	120.6 (5)	C(6)–C(5)–H(4)	108 (3)
C(3)–C(4)–C(5)	120.1 (4)	C(5)–C(6)–H(5)	116 (3)
C(4)–C(5)–C(6)	120.1 (5)	C(1)–C(6)–H(5)	123 (3)
C(5)–C(6)–C(1)	119.7 (4)	C(7)–N—H(6)	130 (4)
C(1)–C(7)–N	117.9 (4)	C(8)–N—H(6)	103 (4)
C(1)–C(7)–O(1)	120.6 (4)	N—C(8)–H(7)	108 (3)
N—C(7)–O(1)	121.5 (4)	C(9)–C(8)–H(7)	119 (3)
C(7)–N—C(8)	121.2 (4)	N—C(8)–H(8)	109 (3)
N—C(8)–C(9)	112.5 (4)	C(9)–C(8)–H(8)	111 (3)
C(8)–C(9)–O(2)	127.0 (4)	H(7)–C(8)–H(8)	96 (5)
C(8)–C(9)–O(3)	108.9 (4)	C(9)–O(3)–H(9)	113 (5)
O(2)–C(9)–O(3)	124.1 (4)		

twofold screw axis parallel to the *a* axis. The molecules are further held together by a N–H...O hydrogen bond to the peptide oxygen atom in the *c* axis screw-related molecule. The molecules are oriented with their long dimension essentially parallel to the *b* axis with the non-carboxyl parts of the molecule tilted about 35° with respect to the (100) plane. The molecular arrangement can be seen in Fig. 1.

Molecular structure

The labelling and the thermal displacement ellipsoids of the atoms can be seen in Fig. 2 and the final positional and vibrational parameters in Table 2. From these values the interatomic distances and angles have been calculated and they are shown in Fig. 3, and are shown together with their estimated standard deviations in Table 3. The root-mean-square components of thermal displacement along the three principal axes are tabulated in Table 4 together with the angles between these principal axes and the unit-cell axes.

The configuration of the molecule is in agreement with earlier structure determinations on similar structures. Compared with the structure of *N*-acetyl glycine, CH₃.CO.NH.CH₂.COOH (Carpenter & Donohue, 1950) the average deviations for comparable non-hydrogen bond lengths and angles are 0.008 Å and 1.3° respectively and no single deviation is significant. The dimensions of the peptide part of the molecule are in relatively good agreement with the averaged values given by Marsh & Donohue (1967). In this case the

mean deviations for bonds and angles are 0.006 Å and 1.3° respectively. The benzene ring has a normal configuration with an average aromatic C–C bond length of 1.397 Å.

The least-squares planes of the structure

Table 5 shows some least-squares planes calculated through the molecule including only non-hydrogen atoms given equal weight. In the benzene ring (plane I) none of the atoms deviates more than 0.005 Å and that part is accordingly perfectly planar within the experimental error. The significant deviations of the atoms from planarity in the peptide (plane II) and carboxyl (plane III) planes depends essentially on the N–C(8) bond which deviates from both of these planes.

The twist of the molecule can be described in terms of two rotations in the same direction. The peptide plane (plane II) is rotated 14° with respect to the benzene ring (plane I) and the carboxyl group (plane III) 83° with respect to the peptide group. The rotations are around the C(1)–C(7) and N–C(8) bonds respectively.

Hydrogen bonding

Both available non-carbon-bonded hydrogen atoms are involved in hydrogen bonds to the peptide oxygen atom. This is demonstrated in Fig. 1 and the distances and angles involved are tabulated in Table 6. The N–H...O bond (3.01 Å) thus connects the molecules forming infinite rows along the *c* axis and the O–H...O

Table 4. *Principal axes (i) of anisotropic temperature factors, referred to the crystallographic axes ABC*The r.m.s. displacements $\bar{\mu}_i$ are in Å and the direction angles, V , are in degrees.

	<i>i</i>	$\bar{\mu}_i$	σ	V_a	σ	V_b	σ	V_c	σ
O(1)	1	0.160	5	71	3	131	5	48	5
	2	0.195	5	91	6	45	6	45	6
	3	0.228	4	161	3	104	5	77	5
O(2)	1	0.179	6	135	6	54	9	67	4
	2	0.202	5	61	8	36	9	109	4
	3	0.292	5	60	2	87	2	31	2
O(3)	1	0.164	5	100	8	169	8	87	4
	2	0.193	5	30	4	100	8	117	3
	3	0.265	5	62	3	92	2	28	3
N	1	0.162	6	106	7	158	10	76	16
	2	0.177	6	101	11	102	16	164	15
	3	0.203	5	160	7	72	6	83	11
C(1)	1	0.162	7	61	11	86	13	29	11
	2	0.165	6	148	33	75	86	63	22
	3	0.186	6	78	75	16	83	101	41
C(2)	1	0.173	6	92	14	171	11	81	14
	2	0.190	7	135	9	95	18	135	10
	3	0.219	7	135	9	82	6	46	9
C(3)	1	0.169	7	79	6	165	7	79	5
	2	0.218	7	30	15	75	7	64	15
	3	0.238	7	118	15	85	6	29	14
C(4)	1	0.174	6	93	14	176	8	93	5
	2	0.199	6	14	7	92	14	104	6
	3	0.250	7	76	6	93	4	14	6
C(5)	1	0.173	7	110	9	147	6	115	5
	2	0.209	7	20	9	109	9	98	9
	3	0.243	7	91	9	116	5	26	5
C(6)	1	0.177	7	122	11	143	13	107	13
	2	0.199	7	111	33	59	20	141	36
	3	0.206	7	140	23	72	23	56	37
C(7)	1	0.158	6	154	9	86	24	64	10
	2	0.170	5	90	23	10	19	100	19
	3	0.187	6	64	9	81	17	27	10
C(8)	1	0.162	7	87	11	174	8	95	6
	2	0.189	6	11	12	86	11	101	12
	3	0.217	6	79	12	95	6	12	11
C(9)	1	0.172	6	89	13	165	14	75	14
	2	0.192	6	110	54	104	15	155	44
	3	0.198	6	160	53	87	18	71	52

Table 5. *Equations of some least-squares planes in the hippuric acid molecule and the distances of the atoms from these planes*Equations are expressed in the form $lA + mB + nC = D$ where A , B , C and D are in Å and A , B and C are along the crystallographic axes respectively.

Plane	Atoms in plane	<i>l</i>	<i>m</i>	<i>n</i>	<i>D</i>
I	C(1), C(2), C(3), C(4), C(5), C(6)	0.8070	-0.0975	0.5824	5.4172
II	C(1), C(7), C(8), N, O(1)	0.9257	-0.0988	0.3651	3.8232
III	C(8), C(9), N, O(2), O(3)	-0.4774	0.0360	0.8779	5.7560
	Plane I		Plane II		Plane III
	C(1) -0.005		C(1) 0.014		C(8) -0.052
	C(2) 0.000		C(7) -0.005		C(9) -0.009
	C(3) 0.005		C(8) 0.019		N 0.041
	C(4) -0.005		N -0.023		O(2) -0.013
	C(5) 0.000		O(1) -0.004		O(3) 0.033
	C(6) 0.005				

Table 6. *Some distances and angles involved in the hydrogen bonds*

Donor	Acceptor	Hydrogen	X-H...O	σ	H...O	σ	X-H-O	σ
N	O(1) ($\frac{1}{2}-x$; $1-y$; $z-\frac{1}{2}$)	H(6)	3.011	6	2.30 Å	6	137°	5
O(3)	O(1) ($\frac{1}{2}+x$; $1\frac{1}{2}-y$; $2-z$)	H(9)	2.680	6	1.95	6	166	6

bonds (2.68 Å) connect the molecules in infinite rows along the *a* axis. Together these two hydrogen bonds form a stabilized three-dimensional intermolecular network.

The proposed intramolecular hydrogen bond for hippuric acid in solution (Schätzle & Rottenberg, 1963) between the unprotonized carboxyl oxygen atom and the nitrogen atom is found to be sterically impossible in the solid state.

This work has been supported by the Swedish Medical Research Council (Project No B70 -11X - 144 - 06A).

References

- CARPENTER, G. B. & DONOHUE, J. (1950). *J. Amer. Chem. Soc.* **72**, 2315.
 CRUICKSHANK, D. W. J. (1965). In *Computing Methods in Crystallography*. Oxford: Pergamon Press.
 KARLE, J. & HAUPTMAN, H. (1956). *Acta Cryst.* **9**, 635.
 LINDGREN, O., LINDQVIST, O. & NYBORG, J. (1970). To be published in *Acta Chem. Scand.*
 MARSH, R. E. & DONOHUE, J. (1967). *Advanc. Protein Chem.* **22**, 235.
 RINGERTZ, H. (1969). In *Stereochemical Aspects of Purine Degradation*. Thesis, Stockholm: Tryckeri Balder AB.
 SCHÄTZLE, E. & ROTTENBERG, M. (1963). *Experientia*, **21**, 373.

Acta Cryst. (1971). B27, 291

The Crystal Structure of Disodium Dihydrogen Hypophosphate Hexahydrate ($\text{Na}_2\text{H}_2\text{P}_2\text{O}_6 \cdot 6\text{H}_2\text{O}$) and Disodium Dihydrogen Pyrophosphate Hexahydrate ($\text{Na}_2\text{H}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$)

By R. L. COLLIN AND M. WILLIS

Department of Radiation Biology and Biophysics, School of Medicine and Dentistry, University of Rochester, Rochester, New York 14620, U.S.A.

(Received 3 December 1969)

The crystal structures of the isomorphous disodium hypophosphate hexahydrate ($\text{Na}_2\text{H}_2\text{P}_2\text{O}_6 \cdot 6\text{H}_2\text{O}$) and disodium dihydrogen pyrophosphate hexahydrate ($\text{Na}_2\text{H}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$) have been determined with diffractometer data. The space group is *C2/c* and a unit cell contains four formula units. The unit-cell dimensions of $\text{Na}_2\text{H}_2\text{P}_2\text{O}_6 \cdot 6\text{H}_2\text{O}$ are $a = 14.090$ (3), $b = 6.998$ (1), $c = 12.700$ (6) Å, $\beta = 115.94$ (2)° and those of $\text{Na}_2\text{H}_2\text{P}_2\text{O}_7 \cdot 6\text{H}_2\text{O}$ are $a = 14.099$ (6), $b = 6.959$ (4), $c = 13.455$ (8) Å, $\beta = 117.69$ (4)°. The hypophosphate ion has *C*₂ symmetry with a P-P distance of 2.190 (1) Å. The mean terminal P-O distance is 1.506 (2) Å while the terminal P-O(H) distance is 1.588 (2) Å. The pyrophosphate ion also has *C*₂ symmetry. The bridge P-O-P bonds make an angle of 136.1 (1)° and the P-O (bridge) distance is 1.598 (1) Å. The mean value of the terminal P-O distance is 1.494 (2) Å while the terminal P-O(H) distance is 1.569 (2) Å. The bridge oxygen atom of the pyrophosphate is not involved in any appreciable intermolecular bonding and the packing of the ions is similar in both structures.

Introduction

The unit-cell dimensions and space groups for a number of hydrated sodium hypophosphate and pyrophosphate salts have been reported by Corbridge (1957). In both the tetrasodium decahydrate and disodium dihydrogen hexahydrate series the hypophosphate salt (containing a phosphorus-phosphorus bond) and the pyrophosphate salt (containing a phosphorus-oxygen-phosphorus bridge) have the same space group and similar unit-cell dimensions. Cor-

bridge suggested that these two hypophosphate-pyrophosphate salt pairs were isomorphous and interpreted his preliminary *b* axis projections in the disodium dihydrogen series to indicate that the P-O-P bond in the pyrophosphate was linear with the oxygen atom either on a twofold axis or at a center of symmetry. He found the P-P bond in the hypophosphate to be in a similar orientation.

We have determined the crystal structures with diffractometer data of both the disodium dihydrogen hypophosphate hexahydrate ($\text{Na}_2\text{H}_2\text{P}_2\text{O}_6 \cdot 6\text{H}_2\text{O}$) and