

## The Crystal Lattice of Sodium Bicarbonate, $\text{NaHCO}_3$

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Citation: [The Journal of Chemical Physics](#) **1**, 634 (1933); doi: 10.1063/1.1749342

View online: <http://dx.doi.org/10.1063/1.1749342>

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## The Crystal Lattice of Sodium Bicarbonate, $\text{NaHCO}_3$

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(Received June 5, 1933)

### I. INTRODUCTION

SOME time ago we started in this laboratory crystal structure examinations of the bicarbonates of ammonium, potassium and sodium. The investigations were undertaken in the hope that some results might be obtained concerning the rôle which the hydrogen atoms play in salts of polybasic acids.

The ammonium compound is orthorhombic and some preliminary results obtained on this crystal have already been published from this laboratory.<sup>1</sup> The bicarbonates of potassium and sodium are monoclinic, but not isomorphous with each other.

Crystals of sodium bicarbonate are described in Groth, *Chemische Krystallographie*.<sup>2</sup> The symmetry is given as monoclinic prismatic with the following elements:

$$a : b : c = 0.7645 : 1 : 0.3582 \quad \beta = 93^\circ 19'.$$

There is a perfect cleavage parallel to the (101) face, a rather perfect one parallel to the (111) face and an imperfect cleavage parallel to (100).

By slow evaporation of aqueous solutions I obtained small but excellent crystals of  $\text{NaHCO}_3$ . They were needle-shaped parallel to the crystallographic  $c$ -axis. Twinned crystals were often observed; the two individuals having the (101) face in common. Dr. Tom. Barth of the Geophysical Laboratory was kind enough to examine my crystals optically. He found that the birefringence was strong and negative in character. The refractive indices were found to be:

$$\alpha = 1.38 \pm 0.01 \quad \beta = 1.50 \pm 0.01 \quad \gamma = 1.58 \pm 0.01.$$

The plane of the optical axes is (010),  $2V$  being  $102^\circ$ . The acute bisectrix is exactly normal to the cleavage plane (101). More accurate values

for the refractive indices are:

$$\alpha = 1.380 \quad \beta = 1.500 \quad \gamma = 1.586.^3$$

All the x-ray observations were taken on one crystal of approximate dimensions  $0.3 \times 0.2 \times 1.0$  mm. A series of Laue photographs and a large number of oscillation photographs were taken. The Laue photographs served merely as a check on the size of the unit cell, as the intensity considerations were based entirely on the observations obtained from the oscillation photographs. For the latter Mo  $K\alpha$  radiation was used. The wave-length of the  $\alpha_1\alpha_2$  doublet was taken to be  $0.7095\text{\AA}$ . The angle through which the crystal was oscillated was for all exposures  $15^\circ$ . Reflections from some 300 different planes were recorded on the photographs.

### II. UNIT CELL AND SPACE GROUP

The dimensions of the unit cell were found to be:

$$\begin{aligned} a &= 7.51 \pm 0.04\text{\AA} & c &= 3.53 \pm 0.03\text{\AA} \\ b &= 9.70 \pm 0.04\text{\AA} & \beta &= 93^\circ 19'. \end{aligned}$$

The cell dimensions correspond to the axial ratios  $0.774 : 1 : .364$ .

The density is given by Groth as 2.221, in *International Critical Tables* as 2.20. Consequently there are four molecules of  $\text{NaHCO}_3$  in the unit cell. The calculated density is  $2.16 \pm 0.04$ .

According to the observed symmetry the space group must belong to the monoclinic prismatic class. As reflections from planes for which  $h+k$  and  $k+l$  are odd have been observed, the translation lattice is simple monoclinic.

Reflections  $h0l$  are absent if  $h+l$  is odd and reflections  $Ok0$  are absent in odd orders. Consequently the symmetry plane is a glide plane with translations  $a/2 + c/2$  rather than a reflection plane, and the twofold axis is a screw axis

<sup>1</sup> R. C. L. Mooney, *Phys. Rev.* **39**, 861 (1932).

<sup>2</sup> P. v. Groth, *Chemische Krystallographie* II, 191, Leipzig, 1908.

<sup>3</sup> H. Brasseur, *Zeits. f. Krist.* **83**, 493 (1932).

rather than a simple rotation axis. Because of the large number of atoms in the unit cell, it may be safely assumed that at least some of them occupy general positions in the space group. It follows that the correct space group is  $P2_1/n(C_{2h}^5)$ .

The positions of this space group referred to a center of symmetry as origin become:

Centers of symmetry:

$$(000)(\frac{1}{2}0\frac{1}{2}), (\frac{1}{2}00)(00\frac{1}{2}), (0\frac{1}{2}0)(\frac{1}{2}\frac{1}{2}\frac{1}{2}), (\frac{1}{2}\frac{1}{2}0)(0\frac{1}{2}\frac{1}{2})$$

General positions:  $\pm(xyz)\pm(x+\frac{1}{2}, \frac{1}{2}-y, z+\frac{1}{2})$ .

The expression for the structure amplitude for atoms in general positions becomes:

$h+k+l$  even

$$F = 4\sum f_n \cos(h2\pi x + l2\pi z) \cos 2\pi yk \quad (1)$$

$h+k+l$  odd

$$F = -4\sum f_n \sin(h2\pi x + l2\pi z) \sin 2\pi yk. \quad (2)$$

### III. DETERMINATION OF THE STRUCTURE

The probable number of degrees of freedom in the structure is 15. In general it is not a hopeless task to determine uniquely an atomic arrangement containing 15 degrees of freedom. It was soon found out, however, that in the present case a direct attack on the structure would lead to extreme difficulties. This circumstance was caused by the fact that all the atoms (neglecting the hydrogen atoms) have appreciable values of the scattering power over the entire range of observations, and also by the fact that all intensities of reflection occurring at small values of  $\sin \theta/\lambda$  were relatively weak.

It is safe to make the assumption that  $\text{CO}_3$ -groups exist in the atomic arrangement. The dimensions of the  $\text{CO}_3$ -group are known rather accurately from previous structure determinations on other carbonates. The group has the shape of an equilateral triangle with the carbon atom at the center and the three oxygen atoms at the corners. The distance from carbon to oxygen is about 1.27Å. Because of the strong forces inside the  $\text{CO}_3$ -group there can be only negligible differences in dimensions as we pass from one crystal to another. I wish to emphasize the fact that in the present case there is no danger in making assumptions of this kind, even

if the assumptions should not happen to be correct. The scattering powers of oxygen as well as of carbon are of the same order of magnitude as that of sodium and it would therefore be impossible to obtain agreement with the observed intensities for a large number of reflections if the assumptions were incorrect. The existence of  $\text{CO}_3$ -groups necessitates that the carbon atoms as well as the oxygen atoms occupy general positions of the space group. Hence the number of parameters for the carbon and oxygen atoms is 12.

It follows from the optical properties that the  $\text{CO}_3$  groups are oriented with their planes parallel to the cleavage face (101) (or very nearly so). In this manner we have reduced the number of parameters for the carbon and oxygen atoms from 12 to 4. Three parameters fix the position of the carbon atom and a fourth one takes care of the rotation of the whole group in the (101) plane.

Let  $x_1y_1z_1$  be the coordinates of the carbon atom expressed in fractions of the cell dimensions and let  $\chi$  be the parameter fixing the rotation of the whole  $\text{CO}_3$ -group in the (101) plane. The value  $\chi=0^\circ$  corresponds to the following orientation of the group: One edge of the equilateral triangle is parallel to the (010) face, the opposite corner of the triangle pointing in the positive direction of the  $b$ -axis. For the sake of convenience we introduce new parameters defined by the relations:

$$\varphi_1 = 2\pi x_1 \quad \varphi_2 = 2\pi y_1 \quad \varphi_3 = 2\pi z_1.$$

The determination of the atomic arrangement was now made in the following straightforward but rather laborious way. The contribution of the  $\text{CO}_3$  group to the amplitude for reflections  $hko$  depends only upon  $\varphi_1$ ,  $\varphi_2$  and  $\chi$ . This contribution was calculated as function of  $\varphi_1$ ,  $\varphi_2$  and  $\chi$  for a large number of reflections  $hko$ . Calculations were made for  $5^\circ$  intervals in  $\varphi_1$  and  $\varphi_2$  and for intervals of  $7\frac{1}{2}^\circ$  in  $\chi$ .

The contribution from the sodium atoms to the structure amplitudes of the same reflections  $hko$  was next calculated on the assumption that the sodium atoms were situated at centers of symmetry. Adding together the contributions we found, however, that agreement with observed intensities could not be obtained for any

set of values  $\varphi_1\varphi_2\chi$ . It was consequently concluded that the sodium atoms have to lie in general positions, characterized by coordinates  $x_2y_2z_2$ . Again we will introduce new parameters defined by the relations  $\psi_1=2\pi x_2$   $\psi_2=2\pi y_2$   $\psi_3=2\pi z_2$ .

The contribution from the sodium atoms to the structure amplitude for reflections  $hkl$  was then calculated as function of  $\psi_1$  and  $\psi_2$ . The calculations were made for intervals of  $5^\circ$  in  $\psi_1$  and  $\psi_2$ .

Combining now the contributions from the  $\text{CO}_3$  groups and the sodium atoms it was found

that agreement with observations could be obtained only for one set of values  $\varphi_1\varphi_2\chi\psi_1\psi_2$ , namely the following:

$$\begin{aligned}\varphi_1 &= 25^\circ & \varphi_2 &= 85^\circ & \chi &= 0^\circ \\ \psi_1 &= 100^\circ & \psi_2 &= 0^\circ\end{aligned}$$

The remaining two parameters,  $\varphi_3$  and  $\psi_3$ , which fix the translation of the sodium and carbon atoms in the direction of the  $c$ -axis, can then be determined very easily and one finds:

$$\varphi_3 = 113^\circ \quad \psi_3 = 255^\circ.$$

TABLE I. Observed intensities and calculated amplitudes.

<i>hkl</i>	$\sin \theta/\lambda$	<i>I</i>	<i>F</i>	<i>hkl</i>	$\sin \theta/\lambda$	<i>I</i>	<i>F</i>	<i>hkl</i>	$\sin \theta/\lambda$	<i>I</i>	<i>F</i>	<i>hkl</i>	$\sin \theta/\lambda$	<i>I</i>	<i>F</i>
110	0.0843	w	-6	420	0.2860	w	20	322	0.3540	w	-12	461	0.4278	nil	3
020	.1031	ms	-13	241	.2872	nil	7	142	.3545	nil	-7	630	.4290	nil	0
120	.1228	w	-4	340	.2873	m	-18	501	.3554	w	16	371	.3329	w	-18
200	.1333	w	-10	012	.2887	vw	14	232	.3555	nil	-2	280	.4334	w-	-12
210	.1430	s	-22	250	.2902	vw	4	351	.3600	nil	0	103	.4348	nil	-2
011	.1511	m	-9	112	.2929	s	39	142	.3601	w	-16	262	.4360	ms	34
101	.1537	m	-32	051	.2943	w	-17	441	.3603	nil	3	081	.4362	nil	-2
101	.1601	s-	-35	331	.2951	nil	0	261	.3628	w	13	461	.4370	nil	6
111	.1621	s-	29	112	.2997	nil	-9	170	.3670	w	-13	113	.4378	nil	-1
111	.1682	vs	-50	411	.2999	s	-42	530	.3675	m	-32	352	.4395	nil	9
130	.1684	s-	-22	151	.3001	nil	-6	261	.3683	w	-5	371	.4398	nil	-2
220	.1686	s	-40	022	.3022	w-	-17	360	.3684	w	-14	181	.4401	vw	-18
021	.1755	vw	-6	151	.3034	m	24	501	.3692	w-	23	181	.4424	w	19
121	.1851	s	-31	122	.3062	vw	13	450	.3709	m-	-17	262	.4452	w	22
121	.1904	vs	64	202	.3074	m-	25	441	.3712	w	10	123	.4469	w	-24
211	.1965	nil	5	430	.3083	nil	-3	332	.3723	s	-41	470	.4487	m	28
230	.2042	vw	-3	060	.3093	vs	57	402	.3792	w	-23	640	.4500	nil	-6
040	.2062	nil	-1	212	.3117	w-	2	242	.3808	m	22	281	.4539	w	-18
211	.2064	vw	-4	122	.3127	nil	9	052	.3836	nil	-1	560	.4547	w-	-10
310	.2065	w	9	421	.3129	nil	-7	270	.3847	w	10	281	.4583	nil	-1
031	.2100	vw-	-2	411	.3130	s	29	152	.3868	w	16	380	.4584	m-	20
221	.2158	s	-44	341	.3158	m-	25	071	.3878	nil	-2	362	.4587	w-	2
140	.2167	vw	11	160	.3164	vw	-9	332	.3881	w-	-4	072	.4592	nil	-8
131	.2180	nil	2	251	.3200	w	14	361	.3910	w-	-4	133	.4615	nil	0
131	.2226	nil	1	202	.3202	m-	33	152	.3919	w	-14	172	.4619	m	30
221	.2249	vw-	-2	032	.3235	vw	1	540	.3920	w	-10	172	.4662	nil	-4
320	.2250	vs	48	222	.3242	w-	10	451	.3921	w-	10	471	.4664	s-	-30
301	.2391	w	14	212	.3242	ms	48	171	.3923	w-	-13	190	.4688	w-	-12
311	.2446	w	-6	341	.3251	w	-17	171	.3948	w	-8	710	.4695	w-	15
231	.2447	s	38	421	.3255	w	-19	342	.3965	vw	4	362	.4716	vw	12
240	.2456	s	-36	251	.3262	m-	-25	361	.3986	vw	-19	272	.4740	vw	-2
041	.2504	ms	22	350	.3263	m-	14	402	.3998	w-	-6	471	.4749	m-	21
301	.2514	vs	-57	132	.3272	w	-16	600	.4000	m	-33	650	.4759	vw	2
231	.2528	vw-	10	132	.3333	vw-	-5	252	.4012	nil	1	381	.4767	m	31
330	.2528	s	30	431	.3335	nil	7	451	.4022	w-	10	720	.4780	nil	0
311	.2566	nil	3	222	.3364	w	23	610	.4033	vw	-11	602	.4782	vw	8
141	.2572	s	-28	260	.3368	m	-26	271	.4077	nil	3	143	.4812	w-	-15
321	.2604	w	29	440	.3371	w	19	460	.4084	m	20	272	.4824	nil	7
141	.2610	s	51	510	.3373	w-	-10	252	.4110	w	-32	290	.4828	w-	-11
150	.2663	m	20	061	.3403	w	-18	342	.4114	w-	-12	381	.4830	m	-30
400	.2667	w	27	312	.3426	w-	-8	080	.4124	m	22	091	.4853	nil	0
410	.2716	vw-	8	232	.3441	nil	0	271	.4125	nil	6	191	.4888	w-	14
321	.2717	w	-19	431	.3453	w	-17	370	.4126	vw	6	191	.4908	vw	-8
241	.2802	m-	24	161	.3454	m-	-23	620	.4130	vw	-2	480	.4912	vw	9
002	.2841	s	-41	161	.3482	vw	5	180	.4178	vw	-1	570	.4913	nil	-3
331	.2848	nil	2	520	.3489	w	21	062	.4199	w-	-14	730	.4917	m-	25
042	.3510	w	-18	352	.4256	w	-20	550	.4214	m-	-17	372	.4949	nil	-2
351	.3516	w-	10	162	.4276	w-	15	162	.4229	nil	-4	701	.4950	nil	-5

The final coordinates of all the atoms are given in Table II. The correctness of our initial assumptions concerning the  $\text{CO}_3$  groups are adequately proved by the fact that good agreement between observed and calculated intensities is obtained. Changes in the size of the  $\text{CO}_3$ -group do not seem to improve the agreement.

The  $f$ -curves used in the calculations are given in Table III. In agreement with modern conceptions of the binding inside the  $\text{CO}_3$ -group I have assumed the states of ionization as  $\text{C}^{+1}$  and  $\text{O}^{-1}$ .

When one compares the calculated structure amplitudes,  $F$ , with the observed intensities,  $I$ , in Table I, the following facts should be kept in mind. If the crystal is of the mosaic type the intensity is proportional to the square of the amplitude, while for ideally perfect crystals the intensity is proportional to the amplitude itself. Aside from the structure amplitude the intensity depends upon a series of factors. The polarization factor, the Lorentz factor and the temperature factor changes continually with increasing values of  $\sin \theta/\lambda$ . Hence they can be left out of consideration if we compare intensities of reflections occurring at similar values of  $\sin \theta/\lambda$ . The absorption can safely be disregarded too, because of the low absorption coefficient and because we used a very small crystal.

TABLE II. Final parameter values.

	In angular measure			In fractions of cell dimensions		
	$2\pi x$	$2\pi y$	$2\pi z$	$x$	$y$	$z$
Na	100°	0°	255°	0.278	0	0.708
C	25°	85°	113°	.069	0.236	.314
O <sub>I</sub>	25°	132°	113°	.069	.367	.314
O <sub>II</sub>	72°	61°	66°	.200	.169	.183
O <sub>III</sub>	338°	61°	160°	.939	.169	.444
H	115°	90°	23°	.319	.250	.064

TABLE III. The scattering powers.<sup>4</sup>

$\sin \theta/\lambda$	0	0.10	0.20	0.30	0.40	0.50	0.60	0.70
$\text{Na}^{+1}$	10	9.5	8.3	6.9	5.4	4.1	3.2	2.6
$\text{C}^{+1}$	5	3.6	2.5	2.0	1.9	1.7	1.6	1.4
$\text{O}^{-1}$	9	7.9	5.9	4.2	2.9	2.2	1.8	1.6

#### IV. DISCUSSION OF THE STRUCTURE

A projection of the atomic arrangement is reproduced in Fig. 1.

<sup>4</sup> James and Brindley, Zeits. f. Krist. **78**, 470 (1931).

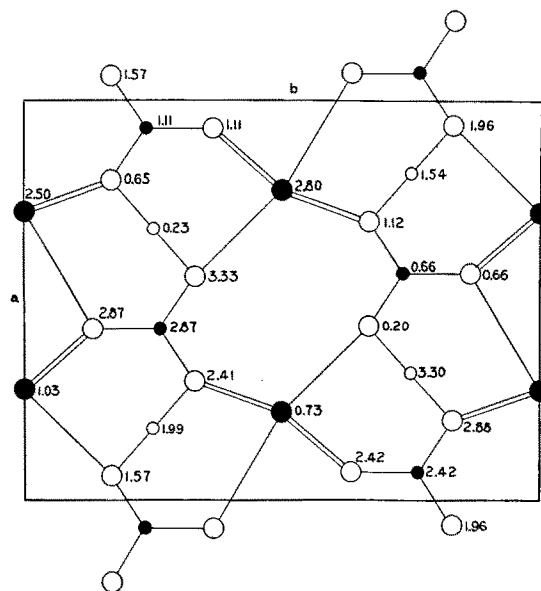


FIG. 1. The atomic arrangement in sodium bicarbonate. The figure shows the atomic arrangement viewed along the  $c$ -axis. Large open circles represent oxygen atoms, large filled circles sodium atoms, small open circles hydrogen atoms and small filled circles represent the carbon atoms. Bonds between atoms are indicated by connection lines. The attached numbers represent the heights in Å above the  $c$ -face. It should be remembered that since the crystal is monoclinic the  $c$ -face is not normal to the  $c$ -axis. In the figure the  $c$ -face passes through the two horizontal edges, of which the upper one lies in the plane of the paper, while the lower one lies below the plane of the paper an amount 0.43Å.

Each sodium atom is surrounded by 6 oxygen atoms in the first sphere of coordination. Of these six oxygen atoms three are of the type O<sub>I</sub>, two are of the type O<sub>II</sub>, while there is only one of the type O<sub>III</sub>. The distance from sodium to the different oxygen atoms is:

Na—O <sub>I</sub>	2.55Å	Na—O <sub>II</sub>	2.44Å
—O <sub>I</sub>	2.37Å	—O <sub>II</sub>	2.53Å
—O <sub>I</sub>	2.57Å	—O <sub>III</sub>	2.35Å

The average Na—O distance is thus 2.47Å, which compares favourably with the value 2.44Å calculated on the basis of the ionic radii published by the author.<sup>5</sup> Goldschmidt's<sup>6</sup> and Pauling's<sup>7</sup> values for the Na—O distance are 2.30Å and 2.35Å, respectively. In other crystals where sodium occurs with coordination number six,

<sup>5</sup> W. H. Zachariasen, Zeits. f. Krist. **80**, 137 (1931).

<sup>6</sup> See V. M. Goldschmidt, Geochem. Verteil. Gesetze d. Elemente **VII**, Vid. Akad. Skr. Oslo (1926).

<sup>7</sup> L. Pauling, J. Am. Chem. Soc. **49**, 763 (1927).

the following Na—O values have been found: In NaClO<sub>3</sub> 2.46Å,<sup>8</sup> in NaNO<sub>2</sub> 2.48Å,<sup>9</sup> in Na<sub>2</sub>SO<sub>4</sub> 2.41Å.<sup>10</sup>

For the distance between oxygen atoms belonging to different CO<sub>3</sub> groups we get the following values: 2.55Å, 3.12Å, 3.15Å, 3.19Å.

### V. THE HYDROGEN BONDS

The positions of the hydrogen atoms cannot be found from intensity calculations. Their location in the atomic arrangement, however, can be found by very simple considerations.

Whereas the binding within the carbonate group presumably comes closer to the valence type than to the ionic type, it must be assumed that the bonds between sodium and oxygen atoms are chiefly ionic in character. This conclusion is confirmed by the fact that the co-ordination number around sodium as well as the observed sodium to oxygen distance can be correctly calculated from the (univalent) ionic radii of 0.98Å and 1.76Å for Na<sup>+</sup> and O<sup>-2</sup>.<sup>4</sup> The effective radius of the oxygen ion in the coordination sphere around sodium is 1.57Å. (Compare the author's paper on ionic radii.) The smallest distance to expect between two oxygen ions in the coordination sphere around sodium is consequently 3.14Å. All the oxygen to oxygen distances except the one of 2.55Å between an O<sub>II</sub> and an O<sub>III</sub> atom are in harmony with this result. The small distance of 2.55Å has to be attributed to the fact that additional binding forces are operative between oxygen atoms O<sub>II</sub> and O<sub>III</sub>. This additional binding has to be ascribed to the presence of a hydrogen atom (ion). We thus come to the conclusion that the hydrogen atoms are located halfway between oxygen atoms O<sub>II</sub> and O<sub>III</sub>, forming a group O—H—O with a distance of 1.275Å between a hydrogen and an oxygen atom.

One gets additional support for this location of the hydrogen atoms by applying Pauling's principle of balanced valence.<sup>11</sup> The sum of the strength of the sodium and carbon bonds ending upon the different kinds of oxygen atoms are

<sup>8</sup> W. H. Zachariasen, *Zeits. f. Krist.* **71**, 517 (1929).

<sup>9</sup> G. E. Ziegler, *Phys. Rev.* **38**, 1040 (1931).

<sup>10</sup> W. H. Zachariasen and G. E. Ziegler, *Zeits. f. Krist.* **81**, 192 (1932).

<sup>11</sup> L. Pauling, *J. Am. Chem. Soc.* **51**, 1010 (1929).

1.83 for O<sub>I</sub>, 1.67 for O<sub>II</sub> and 1.50 for O<sub>III</sub>. In order to bring the total sum of the bond strengths for each oxygen atom as close to 2.00 as possible it becomes necessary to link up the atoms O<sub>II</sub> and O<sub>III</sub> each to one hydrogen atom. But this is exactly what we found above in another way. The total bond strengths become 1.83 for O<sub>I</sub>, 2.17 for O<sub>II</sub> and 2.00 for O<sub>III</sub>.

When we say that the hydrogen atoms lie halfway between two oxygen atoms O<sub>II</sub> and O<sub>III</sub>, we mean the time average positions. It is, of course, conceivable that the hydrogen atom part of the time may be closer associated with atom O<sub>II</sub>, part of the time closer associated with atom O<sub>III</sub>, i.e., that the hydrogen atom oscillates back and forth between the two oxygen atoms.

In his structure investigation of KH<sub>2</sub>PO<sub>4</sub>, J. West<sup>12</sup> was led to the conclusion that the hydrogen atoms also in that compound were situated halfway between two oxygen atoms. For the H—O distance West gives 1.27Å, in complete agreement with our value. The existence of groups (O—H—O)<sup>-3</sup> in several silicates has been strongly advocated by L. Pauling from considerations based upon his principle of balanced valence. The H—F distance in the analogous hydrofluoric group (F—H—F)<sup>-</sup> is 1.18Å.

It may be mentioned that also in boric acid, H<sub>3</sub>BO<sub>3</sub>, the hydrogen atoms lie halfway between two oxygen atoms.<sup>13</sup> It seems therefore to be a general rule that the hydrogen atoms in crystalline acids and acid salts of oxygen acids form groups (O—H—O), the two oxygen atoms belonging to different radicals. In acids like H<sub>3</sub>PO<sub>3</sub> and H<sub>3</sub>PO<sub>2</sub> the formulae have to be written as H<sub>2</sub>(HPO<sub>3</sub>) and H(H<sub>2</sub>PO<sub>2</sub>), so that compounds R<sub>2</sub>(HPO<sub>3</sub>) and R(H<sub>2</sub>PO<sub>2</sub>) are not to be termed acid salts. A compound like NH<sub>4</sub>(HPO<sub>3</sub>)H, however, is a true acid salt, in which there exist groups O—H—O. For bisulphites the formulae probably have to be written as R(SO<sub>3</sub>)H, although it is conceivable that the hydrogen atom might be attached directly to the sulphur atom, R(HSO<sub>3</sub>). Careful x-ray examinations of bisulphites would settle that question.

In the NaHCO<sub>3</sub> structure the hydrogen atoms

<sup>12</sup> J. West, *Zeits. f. Krist.* **74**, 306 (1930).

<sup>13</sup> From unpublished data by the author.

link the carbonate groups together so as to form endless strings parallel the  $[10\bar{1}]$  direction. The strings are furthermore flat, their plane being parallel to the (101) face. It is worth noticing that the crystals show a perfect cleavage parallel to the plane of the strings. The bonds between hydrogen and oxygen atoms are, however, not strong enough to give the crystals a fibrous character.

## VI. SUMMARY

Crystals of sodium bicarbonate,  $\text{NaHCO}_3$ , are monoclinic prismatic. The unit cell contains four molecules and has dimensions

$$a = 7.51 \pm 0.04\text{Å} \quad b = 9.70 \pm 0.04\text{Å} \quad c = 3.53 \pm 0.03\text{Å}$$

with an angle  $\beta$  of  $93^\circ 19'$ . The calculated density is 2.16 as against 2.20–2.22 observed. The space group is  $P2_1/n$ .

It was assumed that the lattice contains  $\text{CO}_3$ -groups of the same shape and dimensions as in other carbonates. The optical properties showed that the carbonate groups were oriented

parallel to the (101) face. Starting out from these assumptions all atomic positions (except those for hydrogen) were determined from intensity calculations. The positions of the hydrogen atoms were found from considerations of interatomic distances.

All atoms are lying in general positions in the arrangement:  $\pm(xyz) \pm(x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2})$ . The values of the 18 parameters involved are:

	<i>x</i>	<i>y</i>	<i>z</i>		<i>x</i>	<i>y</i>	<i>z</i>
Na	0.278	0	0.708	OII	0.200	0.169	0.183
C	0.069	0.236	0.314	OIII	0.939	0.169	0.444
OI	0.069	0.367	0.314	H	0.319	0.250	0.064

Each sodium atom is surrounded by six oxygen atoms at an average distance of 2.47Å.

Each hydrogen atom is linked to two oxygen atoms, forming a collinear group O–H–O. The distance H–O is 1.275Å. This result is an additional proof that hydrogen is capable of forming two bonds.

In conclusion I wish to thank Dr. Tom. Barth of the Geophysical Laboratory for the optical examination of my crystals.