We compare observed and calculated neutron diffraction intensities in Table 2.

Table 2. *Neutron diffraction intensities*

hkl	Calculated relative intensities for each distribution I	II	III	Observed intensities
111	282	40	21	323
200	26	241	142	15
220	468	699	832	468
311	237	33	17	208

The formula and coherent scattering amplitudes of Shull & Wollan (1956) were used in calculating intensities. No temperature factors or absorption corrections were included. On the basis of this neutron diffraction data we ascribe the $L2_1$ structure type to $LiMg_2Tl$.

Semiconducting properties are predicted for the compound from the criteria of Mooser & Pearson (1957), and the ^7Li nuclear magnetic resonance line is narrow as it is in other semiconducting lithium intermetallic compounds (Holder, 1964).

I am indebted to Mr. D. H. Wood for some of the sample preparation, to Mr. V. G. Silveira for X-ray diffraction data, to Mr. T. T. Komoto for neutron diffraction data, and the Laboratory's Analytical Chemistry Group for confirmatory analyses.

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Sodium bicarbonate and its hydrogen atom.*

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A recent reinvestigation of the crystal structure of sodium bicarbonate has been described by Sass & Scheuerman (1962). We have used this interesting and relatively simple structure to test certain phases of the least-squares and Fourier sub-programs of our IBM 7094-7040 crystallographic system CRYRM (Duchamp, 1964). In so doing we have not only confirmed the results of Sass & Scheuerman but have also obtained evidence for the position of the hydrogen atom.

We have carried out a number of diagonal, block-diagonal and full-matrix least-squares refinement cycles, based

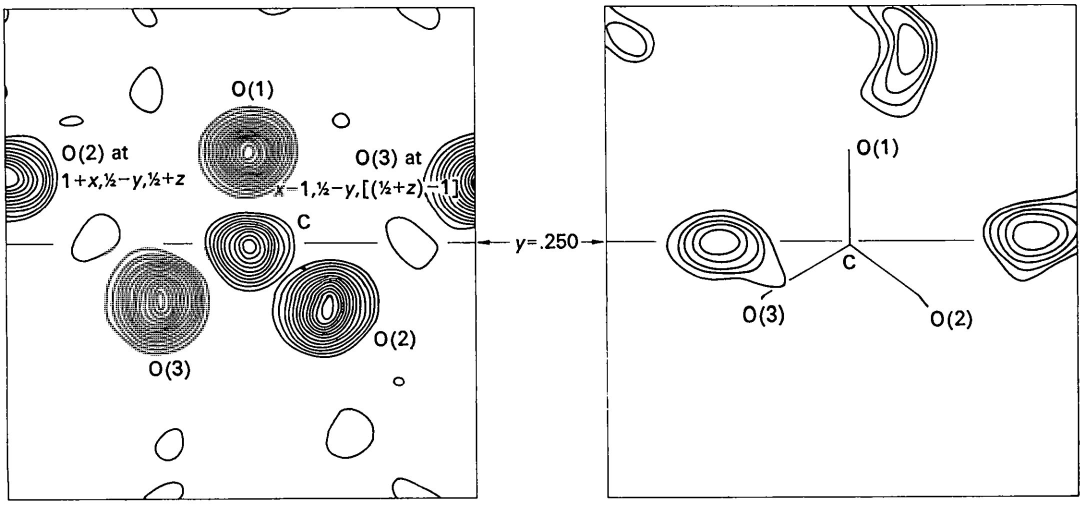

Fig. 1. The electron density map and the difference map in the plane of the bicarbonate ion. The contours for the electron density map are at intervals of 1 e.Å^{-3} beginning with 1 e.Å^{-3}. The contours for the difference map begin with 0·2 e.Å^{-3} and are at intervals of 0·1 e.Å'^{3}. The least-squares position of the hydrogen atom is 0·1 Å out of the plane of the bicarbonate ion. Its height in the three-dimensional difference map (0·9 Å^{-3}) is higher than any other peak.

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Table 1. *The atomic parameters and their standard deviations*

The heavy atom values have been multiplied by 10^4. The temperature factors are in the form $T = \exp(-B_{11}h^2 - B_{22}k^2 - B_{33}l^2 - B_{12}kl - B_{13}hl - B_{23}kl)$. The hydrogen parameters have been multiplied by 10^3. The hydrogen atom was assigned arbitrarily an isotropic B value of 2·0 Å^2.

Atom	$x(\sigma_x)$	$y(\sigma_y)$	$z(\sigma_z)$	$B_{11}(\sigma_{B_{11}})$	$B_{22}(\sigma_{B_{22}})$	$B_{33}(\sigma_{B_{33}})$	$B_{12}(\sigma_{B_{\bar{1}2}})$	$B_{13}(\sigma_{B_{13}})$	$B_{23}(\sigma_{B_{23}})$
Na^+	4285(8)	44(2)	−2855(3)	421(60)	26(3)	72(5)	−19(11)	228(22)	−3(4)
C	2123(20)	2384(6)	−767(5)	369(116)	30(5)	39(8)	2(26)	233(46)	9(9)
O(1)	1893(14)	3666(4)	−714(4)	410(88)	19(4)	57(7)	32(19)	100(34)	−1(6)
O(2)	−104(15)	1619(4)	−2046(5)	321(80)	28(4)	46(7)	−20(18)	89(32)	−33(6)
O(3)	4959(15)	1705(4)	592(5)	550(88)	24(4)	48(7)	35(21)	71(31)	21(7)
H	669(32)	252(10)	143(13)						

Table 2. *Interatomic distances and angles**

Distances	
C–O(1)	1·249 Å
C–O(2)	1·275
C–O(3)	1·345
O(3)–H	1·07
O(3) · · · O(2′)	2·611
H · · · O(2′)	1·56
Na^+ · · · O(1′)	2·477
Na^+ · · · O(1″)	2·442
Na^+ · · · O(1‴)	2·464
Na^+ · · · O(2″)	2·385
Na^+ · · · O(2)	2·425
Na^+ · · · O(3′)	2·432

Angles	
O(1)–C–O(2)	125·5°
O(1)–C–O(3)	119·9
O(2)–C–O(3)	114·6
H–O(3)–C	103·1
C–O(3) · · · O(2′)	112·1
O(3)–H · · · O(2′)	165
O(1′) · · · Na^+ · · · O(1″)	84·5
O(1′) · · · Na^+ · · · O(1‴)	84·0
O(1′) · · · Na^+ · · · O(2″)	83·6
O(1′) · · · Na^+ · · · O(2)	84·3
O(1′) · · · Na^+ · · · O(3′)	162·6
O(1″) · · · Na^+ · · · O(1‴)	91·4
O(1″) · · · Na^+ · · · O(2″)	168·1
O(1″) · · · Na^+ · · · O(2)	86·0
O(1″) · · · Na^+ · · · O(3′)	78·5
O(1‴) · · · Na^+ · · · O(2″)	86·4
O(1‴) · · · Na^+ · · · O(2)	168·2
O(1‴) · · · Na^+ · · · O(3′)	92·5
O(2″) · · · Na^+ · · · O(2)	93·7
O(2″) · · · Na^+ · · · O(3′)	113·2
O(2) · · · Na^+ · · · O(3′)	98·2

*O(1′) at $x, \frac{1}{2}-y, z-\frac{1}{2}$
O(1″) at $\bar{x}, y-\frac{1}{2}, -(\frac{1}{2}+z)$
O(1‴) at $1-x, y-\frac{1}{2}, -(\frac{1}{2}+z)$
O(2′) at $1+x, \frac{1}{2}-y, \frac{1}{2}+z$
O(2″) at $1+x, y, z$
O(3′) at $1-x, \bar{y}, \bar{z}$

on the observed structure factors of Sass & Scheuerman (their Table 1) and beginning with their final parameters (their Table 2); after the first three cycles, the temperature factors were allowed to become anisotropic. The quantity minimized was $\Sigma w(F_o^2 - k^2F_c^2)^2$. Several weighting schemes were tested; in the final cycles function $\sqrt{w} = 1/(0{\cdot}5 - 0{\cdot}5F_o - 0{\cdot}1F_o^2)$ was used, where the denominator expresses our subjective estimate of the usual pattern of uncertainty in F_o^2. Form factors for Na^+, C, and O were taken directly from *International Tables for X-ray Crystallography* (1962); for atoms O(1) and O(2), form factors for $O^{\frac{1}{2}-}$ were taken as the average of O and O^-. Calculation time for one cycle of full-matirx least-squares refinement, with 383 reflexions* and 46 parameters, was 20 seconds.

A three-dimensional difference map, a difference map and an electron density map in the plane of the bicarbonate ion, and a difference projection down the a axis were then calculated. These maps, two of which are shown in Fig. 1, clearly showed the location of the hydrogen atom. A full-matrix least-squares refinement of its coordinates together with the parameters of the heavy atoms led to the final set of parameters, and their standard deviations, listed in Table 1. The final R index was 0·091 and the scale factor $1/k$ to be applied to the observed values of Sass & Scheuerman was 0·926.

Bond distances and angles are listed in Table 2; they do not differ significantly from those of Sass & Scheuerman. The values for the C–O(1) and C–O(2) distances differ from one another by slightly less than three standard deviations; it is interesting to note that the longer distance involves O(2), the acceptor atom of a strong hydrogen bond from O(3). The hydrogen bond, 2·611 Å in length, is clearly not symmetrical.

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* The reflexions 060, 022, 023, 131, $\bar{1}22$, $\bar{1}12$, $\bar{1}04$, and $\bar{2}14$ were given zero weight, as they were presumed to be affected by secondary extinction.