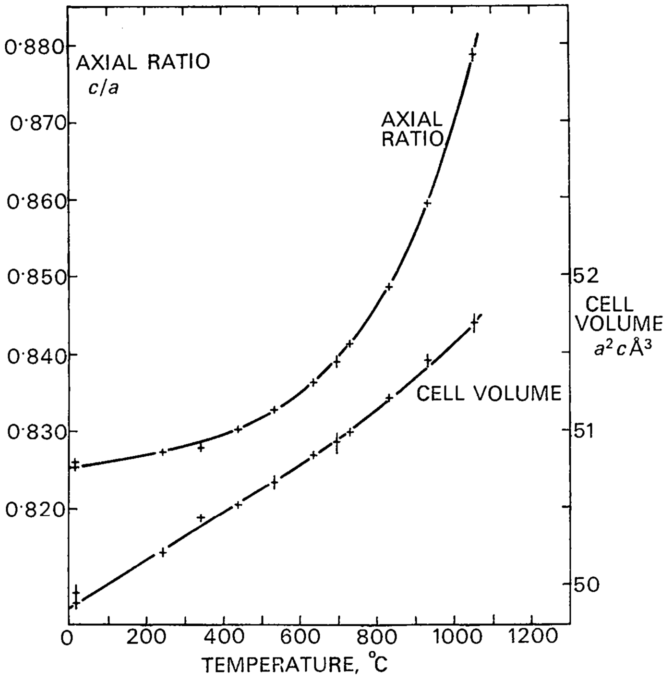

Fig. 2. Axial ratio and cell volume *versus* temperature.

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$LiMg_2Tl$: preparation and structure*.

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A previously unreported compound, $LiMg_2Tl$, is interesting because of its ordered $L2_1$ structure type. We prepared the compound to compare its structure and properties with those of Li_2MgPb (Ramsey, 1961; Ramsey, Sands & Mead, 1963).

The compound was prepared in an Armco iron crucible in an argon atmosphere by melting together weighed amounts of the elements of greater than 99·5% purity. Slight excesses of lithium and magnesium were added to compensate for oxidation. Cooling curves showed that the compound melts congruently at approximately 594 °C. The solid has a grey metallic color, is brittle, and tarnishes in laboratory air in several minutes. The analysis of the material used in these studies was: Li, 26; Mg, 52; Tl, 22 at.%.

X-ray powder patterns of this material, taken with Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å), showed only a single, face-centered cubic phase with $a_0 = 6{\cdot}83_7$ Å. Neutron diffraction measurements on a powdered sample were necessary to establish the positions of the lighter elements within the unit cell. These measurements were carried out in a previously described (Mead & Sparks, 1960) apparatus. While X-ray patterns indicated a single f.c.c. phase, the neutron diffraction spectrum showed, in addition, two very weak lines from an impurity. From their positions, these impurity lines were tentatively ascribed to a trace of either magnesium metal or magnesium metal containing lithium in solid solution.

Taking the positions of the Tl atoms to be at (0,0,0) in the face-centered cubic lattice, the distributions of the lighter elements might occur as shown in Table 1.

Table 1. *Possible distributions of* Li *and* Mg *in* $LiMg_2Tl$

Position	Distribution		
	I	II	III
$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	Li	Mg	$\frac{1}{3}$ Li, $\frac{2}{3}$ Mg
$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}; \frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	2 Mg	Mg, Li	$\frac{2}{3}$ Li, $\frac{4}{3}$ Mg

Distribution I corresponds to the $L2_1$ Heusler alloy type, while distributions II and III correspond to possible disordering.

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* This work was performed under the auspices of the United States Atomic Energy Commission.

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

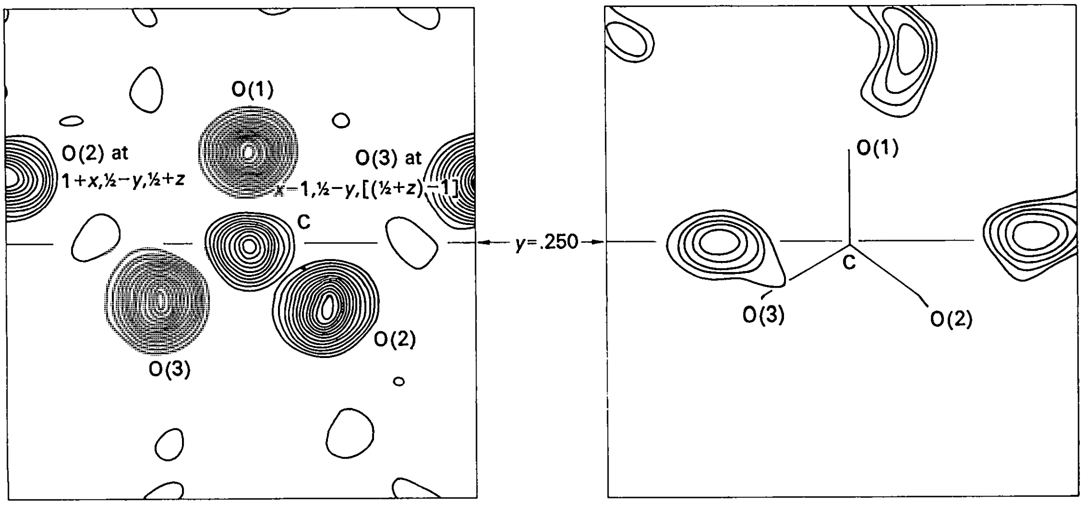

Fig. 1. The electron density map and the difference map in the plane of the bicarbonate ion. The contours for the electron density map are at intervals of 1 e.Å^{-3} beginning with 1 e.Å^{-3}. The contours for the difference map begin with 0·2 e.Å^{-3} and are at intervals of 0·1 e.Å$'^{3}$. The least-squares 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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