be multiplied by the factor of about 8, relating densities on the top to those on the second film, but the intensities will be multiplied by the same factor, so that for this group the error will also be about 0·5% of the greatest intensity measured, corresponding to a nominal density of about 8·0. The lack of uniformity of absorption in the top film will increase this error to about 1·5%.

The contribution to the error from the photometer is negligible over most of the range of density measurement, although, since it is difficult to separate out the two contributions, it is possible that the film error is slightly smaller and the photometer error larger than has been estimated. The main finding, however, is that the total error is small.

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# The Crystal Structure of Nickel β-Alanine Dihydrate*

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Nickel β-alanine dihydrate, $Ni(NH_2CH_2CH_2COO)_2.2H_2O$, crystallized from aqueous solution, is triclinic, space group $P\bar{1}$ with one molecule per unit cell of dimensions

$$a=8{\cdot}48,\ b=6{\cdot}77,\ c=4{\cdot}93\ \text{Å};\ \alpha=103{\cdot}0°,\ \beta=95{\cdot}2°,\ \gamma=102{\cdot}3°.$$

The two nitrogen atoms, the two carboxylic oxygen atoms (one from each β-alanine molecule) and the two water oxygen atoms form a slightly distorted octahedron around the nickel atom. The nickel β-alanine dihydrate units are held together by hydrogen bonds in a stable layer structure parallel to (100). The neighbouring layers are linked with each other by van der Waals bonds.

## Introduction

In a study of β-alanine in this laboratory, a suitable trial structure could not be postulated because of the lack of knowledge of molecular geometry. The present structure analysis of nickel β-alanine dihydrate was undertaken in order to determine the structure of the β-alanine residue, and also because it was of interest to compare its crystal and molecular structure with those of other similar metal complexes. The crystal structure of copper β-alanine hexahydrate has recently been determined (Tomita, 1961).

## Experimental

The crystals of nickel β-alanine dihydrate were obtained from aqueous solution. They are triclinic and grow as needles elongated along the short $c$ axis. The crystal and physical data obtained are as follows:

$$a=8{\cdot}48,\ b=6{\cdot}77,\ c=4{\cdot}93\ \text{Å};$$
$$\alpha=103{\cdot}0°,\ \beta=95{\cdot}2°,\ \gamma=102{\cdot}3°.$$

Space group, $P\bar{1}$.

Preliminary values of axial lengths were obtained by means of rotation photographs, and more accurate values were determined from high-angle axial reflexions in Weissenberg photographs, from which the angles $\alpha$, $\beta$ and $\gamma$ were also obtained.

The observed density at 25 °C, measured by the flotation method, is 1·720 g.cm$^{-3}$, and the calculated density for one molecule of $Ni(NH_2CH_2CH_2COO)_2.2H_2O$ per unit cell is 1·689 g.cm$^{-3}$.

The linear absorption coefficient $\mu$ for Cu $K\alpha$ radiation is 30·1 cm$^{-1}$. Reflexions of the type $hk0$, $h0l$ and $0kl$ were obtained from zero layer Weissenberg photographs, using Cu $K\alpha$ radiation and the multiple film technique. Of the 144 possible reflexions in the $hk0$ zone, 107 were observed, while in the $h0l$ and $0kl$ zones, 73 and 68 reflexions were observed out of a possible 100 and 87 respectively. The specimens used were between about 0·1 mm and 0·25 mm thick along different directions, normal to the oscillation axes. Intensities were measured visually and corrected for the $Lp$ factor in the usual way. No absorption correction was applied.

Preliminary values of the scale factors and the temperature factors, obtained by Wilson's method (1942) were improved during the later stages of

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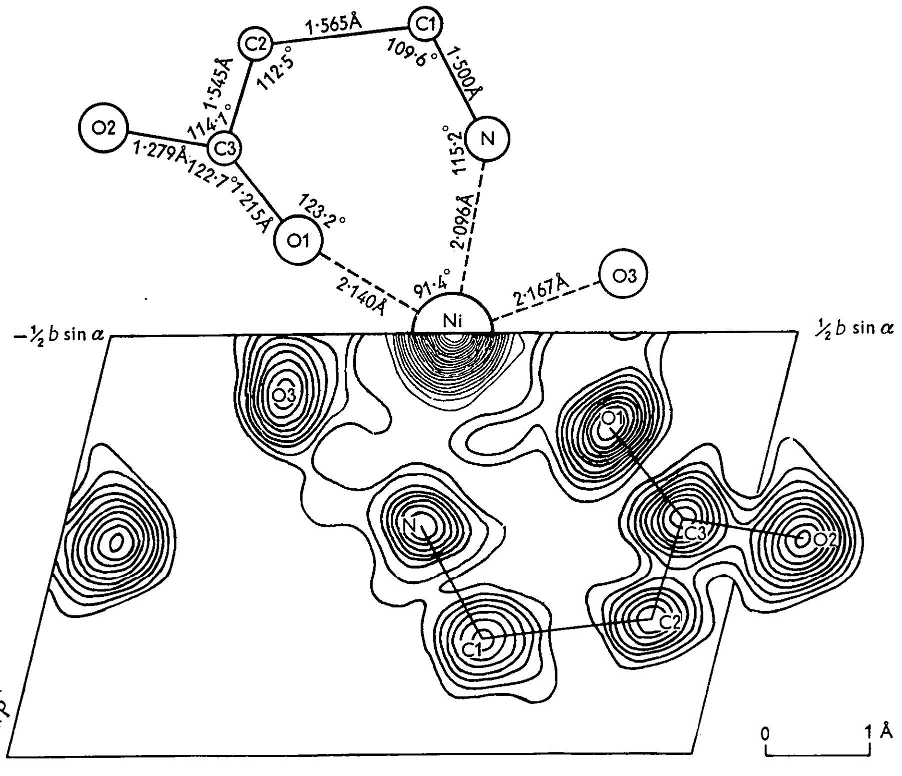

Fig. 1. (001) electron-density projection. Contours at intervals of 2 e.Å$^{-2}$ for Ni and 1 e.Å$^{-2}$ for the other atoms, starting from 2 e.Å$^{-2}$.

refinement. The structure factors were calculated by the use of McWeeny's (1951) values of atomic scattering factors for carbon, nitrogen and oxygen and Thomas & Umeda's (1957) values for $Ni^{2+}$. The atomic scattering factors for $Ni^{2+}$ were corrected for dispersion in the usual way.

## Determination and refinement of the structure

As the space group is $P\bar{1}$ and the nickel atoms lie at the centre of symmetry, the approximate coordinates of the atoms could be directly determined from the three Patterson projections, obtained with the help of the von Eller photosommateur. The atomic coordinates were then refined by repeated difference syntheses. The isotropic temperature factors for all atoms were obtained for each zone by the least squares method. The final values of $R$, on including all except very high-angle unobserved reflexions at half the minimum observable value, were 0·150 for $hk0$, 0·124 for $0kl$ and 0·153 for $h0l$ reflexions. The 001 reflexion appears to be subject to extinction and was excluded from all calculations. The 100, 010 and $\bar{1}10$ reflexions had also to be excluded as they could not be recorded in the photographs.

The (001) electron density projection (Fig. 1) was obtained with calculated signs and $F_o$ values for all except 100, 010 and $\bar{1}10$ reflexions, for which final $F_c$ values were used. The final atomic and thermal parameters are listed in Table 1, and the observed and calculated structure factors in Table 2.

The standard deviations of atomic coordinates and interatomic distances were estimated (Lipson & Cochran, 1953) assuming $p=5$ Å$^2$ and $\sigma(F)/|F|$ to

Table 1. *Final atomic and thermal parameters*

| | $X/a$ | $Y/b$ | $Z/c$ | $B$ ($hk0$) | $B$ ($0kl$) | $B$ ($h0l$) |
|---|---|---|---|---|---|---|
| Ni | 0 | 0 | 0 | 1·8 Å$^2$ | 0·5 Å$^2$ | 1·5 Å$^2$ |
| N | 0·2219 ± 0·0031 | 0·0206 ± 0·0039 | 0·2428 ± 0·0053 | 1·7 | 1·4 | 0·9 |
| C(1) | 0·3675 ± 0·0036 | 0·1638 ± 0·0045 | 0·1813 ± 0·0062 | 2·2 | 1·2 | 2·7 |
| C(2) | 0·3373 ± 0·0036 | 0·3878 ± 0·0045 | 0·2173 ± 0·0062 | 2·9 | 0·8 | 2·6 |
| C(3) | 0·2155 ± 0·0036 | 0·4038 ± 0·0045 | −0·0247 ± 0·0062 | 0·9 | 0·8 | 1·0 |
| O(1) | 0·1095 ± 0·0027 | 0·2555 ± 0·0034 | −0·1631 ± 0·0047 | 2·1 | 1·2 | 2·1 |
| O(2) | 0·2456 ± 0·0027 | 0·5811 ± 0·0034 | −0·0847 ± 0·0047 | 2·3 | 1·3 | 3·2 |
| O(3) | −0·0690 ± 0·0027 | 0·2176 ± 0·0034 | 0·3355 ± 0·0047 | 2·7 | 1·0 | 3·3 |

Table 2. *Observed and calculated structure factors*

| h | k | l | $\lvert F_o\rvert$ | $F_c$ | h | k | l | $\lvert F_o\rvert$ | $F_c$ | h | k | l | $\lvert F_o\rvert$ | $F_c$ | h | k | l | $\lvert F_o\rvert$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 0 | 0 | 6 | -10 | 5 | 4 | 0 | 5 | -3 | $\bar{3}$ | 0 | 1 | 3 | -4 | 0 | 2 | 1 | 21 | 22 |
| 3 | 0 | 0 | 17 | 18 | 6 | 4 | 0 | 3 | 3 | $\bar{4}$ | 0 | 1 | 11 | 8 | 0 | 3 | 1 | 9 | 8 |
| 4 | 0 | 0 | 16 | 16 | 7 | 4 | 0 | 8 | 8 | $\bar{5}$ | 0 | 1 | 10 | 7 | 0 | 4 | 1 | 14 | 14 |
| 5 | 0 | 0 | 12 | 11 | $\bar{1}$ | 4 | 0 | 28 | 30 | $\bar{6}$ | 0 | 1 | 14 | 16 | 0 | 5 | 1 | 17 | 17 |
| 6 | 0 | 0 | < 4 | -1 | $\bar{2}$ | 4 | 0 | 30 | 29 | $\bar{7}$ | 0 | 1 | 10 | 10 | 0 | 6 | 1 | < 4 | -3 |
| 7 | 0 | 0 | 5 | -4 | $\bar{3}$ | 4 | 0 | 3 | 3 | $\bar{8}$ | 0 | 1 | 9 | 9 | 0 | 7 | 1 | 7 | 9 |
| 8 | 0 | 0 | 10 | 10 | $\bar{4}$ | 4 | 0 | 10 | 10 | $\bar{9}$ | 0 | 1 | 10 | 12 | 0 | $\bar{1}$ | 1 | 19 | 22 |
| 9 | 0 | 0 | 13 | 12 | $\bar{5}$ | 4 | 0 | 12 | 13 | 0 | 0 | 2 | < 2 | 1 | 0 | $\bar{2}$ | 1 | 22 | 27 |
| 10 | 0 | 0 | 5 | 2 | $\bar{6}$ | 4 | 0 | 3 | 1 | 1 | 0 | 2 | 18 | 20 | 0 | $\bar{3}$ | 1 | 29 | 32 |
| 1 | 1 | 0 | 9 | 7 | $\bar{7}$ | 4 | 0 | 5 | 5 | 2 | 0 | 2 | 18 | 20 | 0 | $\bar{4}$ | 1 | < 4 | -4 |
| 2 | 1 | 0 | 32 | 36 | $\bar{8}$ | 4 | 0 | 5 | 6 | 3 | 0 | 2 | < 3 | -1 | 0 | $\bar{5}$ | 1 | 14 | 15 |
| 3 | 1 | 0 | 8 | 11 | $\bar{10}$ | 4 | 0 | 6 | 7 | 4 | 0 | 2 | 15 | 14 | 0 | $\bar{6}$ | 1 | 10 | 10 |
| 4 | 1 | 0 | 10 | 11 | 0 | 5 | 0 | 24 | 23 | 5 | 0 | 2 | 17 | 14 | 0 | $\bar{7}$ | 1 | 17 | 16 |
| 5 | 1 | 0 | 24 | 24 | 1 | 5 | 0 | 10 | 10 | 6 | 0 | 2 | < 3 | 2 | 0 | $\bar{8}$ | 1 | 10 | 10 |
| 6 | 1 | 0 | 10 | 11 | 2 | 5 | 0 | 5 | -5 | 7 | 0 | 2 | 6 | 6 | 0 | 1 | 2 | 15 | 9 |
| 7 | 1 | 0 | 8 | 9 | 3 | 5 | 0 | 6 | 7 | 8 | 0 | 2 | 4 | 5 | 0 | 2 | 2 | 26 | 25 |
| 8 | 1 | 0 | 10 | 10 | 4 | 5 | 0 | 14 | 11 | $\bar{1}$ | 0 | 2 | 9 | 9 | 0 | 3 | 2 | < 4 | -4 |
| 9 | 1 | 0 | < 4 | 1 | 5 | 5 | 0 | 8 | 7 | $\bar{2}$ | 0 | 2 | 4 | 5 | 0 | 4 | 2 | 6 | 6 |
| $\bar{2}$ | 1 | 0 | 23 | 25 | 6 | 5 | 0 | 6 | 4 | $\bar{3}$ | 0 | 2 | 18 | 18 | 0 | 5 | 2 | 10 | 11 |
| $\bar{3}$ | 1 | 0 | 24 | 19 | $\bar{1}$ | 5 | 0 | 10 | 10 | $\bar{4}$ | 0 | 2 | 26 | 28 | 0 | 6 | 2 | 6 | 5 |
| $\bar{4}$ | 1 | 0 | 6 | 5 | $\bar{2}$ | 5 | 0 | 9 | 8 | $\bar{5}$ | 0 | 2 | 12 | 13 | 0 | 7 | 2 | 6 | 5 |
| $\bar{5}$ | 1 | 0 | < 3 | 0 | $\bar{3}$ | 5 | 0 | 10 | 11 | $\bar{6}$ | 0 | 2 | 12 | 15 | 0 | $\bar{1}$ | 2 | 10 | -8 |
| $\bar{6}$ | 1 | 0 | 8 | 8 | $\bar{4}$ | 5 | 0 | 10 | 10 | $\bar{7}$ | 0 | 2 | 15 | 17 | 0 | $\bar{2}$ | 2 | 15 | 18 |
| $\bar{7}$ | 1 | 0 | 4 | 5 | $\bar{5}$ | 5 | 0 | 10 | 11 | $\bar{8}$ | 0 | 2 | 6 | 8 | 0 | $\bar{3}$ | 2 | 29 | 33 |
| $\bar{8}$ | 1 | 0 | < 4 | 2 | $\bar{6}$ | 5 | 0 | 3 | -1 | 0 | 0 | 3 | 11 | 8 | 0 | $\bar{4}$ | 2 | < 4 | -1 |
| $\bar{9}$ | 1 | 0 | 5 | 5 | $\bar{7}$ | 5 | 0 | < 4 | -4 | 1 | 0 | 3 | 27 | 32 | 0 | $\bar{5}$ | 2 | < 4 | 0 |
| $\bar{10}$ | 1 | 0 | 8 | 10 | $\bar{9}$ | 5 | 0 | 5 | 6 | 2 | 0 | 3 | 15 | 12 | 0 | $\bar{6}$ | 2 | < 4 | 2 |
| 0 | 2 | 0 | 14 | 13 | 0 | 6 | 0 | < 4 | 1 | 3 | 0 | 3 | < 3 | 2 | 0 | $\bar{7}$ | 2 | 11 | 12 |
| 1 | 2 | 0 | < 2 | 2 | 1 | 6 | 0 | < 4 | -1 | 4 | 0 | 3 | 16 | 15 | 0 | $\bar{8}$ | 2 | 6 | 7 |
| 2 | 2 | 0 | 5 | -2 | 2 | 6 | 0 | 14 | 11 | 5 | 0 | 3 | 14 | 13 | 0 | 1 | 3 | 14 | 12 |
| 3 | 2 | 0 | 13 | 17 | 3 | 6 | 0 | 14 | 12 | 6 | 0 | 3 | 8 | 10 | 0 | 2 | 3 | 14 | 15 |
| 4 | 2 | 0 | 27 | 31 | 4 | 6 | 0 | 6 | 5 | 7 | 0 | 3 | < 2 | 3 | 0 | 3 | 3 | 10 | 10 |
| 5 | 2 | 0 | 18 | 17 | 5 | 6 | 0 | 9 | 7 | $\bar{1}$ | 0 | 3 | < 2 | -2 | 0 | 4 | 3 | 10 | 10 |
| 6 | 2 | 0 | 8 | 9 | $\bar{1}$ | 6 | 0 | 6 | 6 | $\bar{2}$ | 0 | 3 | 13 | 13 | 0 | 5 | 3 | 10 | 8 |
| 7 | 2 | 0 | 10 | 9 | $\bar{2}$ | 6 | 0 | 8 | 7 | $\bar{3}$ | 0 | 3 | 18 | 17 | 0 | 6 | 3 | 6 | 8 |
| 8 | 2 | 0 | < 4 | 4 | $\bar{3}$ | 6 | 0 | 3 | 4 | $\bar{4}$ | 0 | 3 | 22 | 22 | 0 | $\bar{1}$ | 3 | 10 | 9 |
| $\bar{1}$ | 2 | 0 | 5 | 5 | $\bar{4}$ | 6 | 0 | < 4 | 2 | $\bar{5}$ | 0 | 3 | 10 | 9 | 0 | $\bar{2}$ | 3 | 14 | 13 |
| $\bar{2}$ | 2 | 0 | 17 | -15 | $\bar{5}$ | 6 | 0 | 6 | 8 | $\bar{6}$ | 0 | 3 | < 3 | 0 | 0 | $\bar{3}$ | 3 | 12 | 11 |
| $\bar{3}$ | 2 | 0 | 6 | 4 | $\bar{6}$ | 6 | 0 | 10 | 11 | $\bar{7}$ | 0 | 3 | 7 | 8 | 0 | $\bar{4}$ | 3 | 6 | 8 |
| $\bar{4}$ | 2 | 0 | 30 | 32 | $\bar{7}$ | 6 | 0 | 5 | 5 | $\bar{8}$ | 0 | 3 | 5 | 7 | 0 | $\bar{5}$ | 3 | 14 | 15 |
| $\bar{5}$ | 2 | 0 | 24 | 29 | 0 | 7 | 0 | 10 | 9 | 0 | 0 | 4 | 14 | 10 | 0 | $\bar{6}$ | 3 | < 4 | 2 |
| $\bar{6}$ | 2 | 0 | 9 | 11 | 1 | 7 | 0 | 6 | 5 | 1 | 0 | 4 | 14 | 12 | 0 | $\bar{7}$ | 3 | < 4 | 4 |
| $\bar{7}$ | 2 | 0 | < 4 | 3 | 2 | 7 | 0 | < 3 | 2 | 2 | 0 | 4 | < 3 | -1 | 0 | 1 | 4 | 7 | 7 |
| $\bar{8}$ | 2 | 0 | 10 | 11 | 3 | 7 | 0 | 6 | 4 | 3 | 0 | 4 | 6 | 3 | 0 | 2 | 4 | 13 | 15 |
| $\bar{9}$ | 2 | 0 | 12 | 13 | $\bar{1}$ | 7 | 0 | < 4 | 3 | 4 | 0 | 4 | 13 | 10 | 0 | 3 | 4 | 17 | 18 |
| 0 | 3 | 0 | 14 | 16 | $\bar{2}$ | 7 | 0 | < 4 | -2 | 5 | 0 | 4 | 14 | 13 | 0 | 4 | 4 | 5 | 4 |
| 1 | 3 | 0 | 14 | 13 | $\bar{3}$ | 7 | 0 | < 4 | 2 | 6 | 0 | 4 | 14 | 12 | 0 | 5 | 4 | < 2 | 2 |
| 2 | 3 | 0 | 9 | 8 | $\bar{4}$ | 7 | 0 | 8 | 5 | $\bar{1}$ | 0 | 4 | < 3 | -2 | 0 | $\bar{1}$ | 4 | 17 | 17 |
| 3 | 3 | 0 | 9 | 6 | $\bar{5}$ | 7 | 0 | 11 | 10 | $\bar{2}$ | 0 | 4 | 7 | 6 | 0 | $\bar{2}$ | 4 | 17 | 19 |
| 4 | 3 | 0 | 14 | 13 | $\bar{6}$ | 7 | 0 | 6 | 5 | $\bar{3}$ | 0 | 4 | 13 | 11 | 0 | $\bar{3}$ | 4 | 10 | 9 |
| 5 | 3 | 0 | 8 | 9 | 0 | 8 | 0 | 8 | 4 | $\bar{4}$ | 0 | 4 | 11 | 11 | 0 | $\bar{4}$ | 4 | 7 | 6 |
| 6 | 3 | 0 | < 4 | -1 | 2 | 8 | 0 | < 2 | 4 | $\bar{5}$ | 0 | 4 | 15 | 12 | 0 | $\bar{5}$ | 4 | 19 | 20 |
| 7 | 3 | 0 | < 4 | 1 | $\bar{1}$ | 8 | 0 | 9 | 10 | $\bar{6}$ | 0 | 4 | < 3 | 3 | 0 | $\bar{6}$ | 4 | 10 | 9 |
| 8 | 3 | 0 | 6 | 7 | $\bar{2}$ | 8 | 0 | 6 | 5 | $\bar{8}$ | 0 | 4 | 6 | 6 | 0 | $\bar{7}$ | 4 | 6 | 6 |
| $\bar{1}$ | 3 | 0 | 19 | 17 | $\bar{3}$ | 8 | 0 | 6 | 5 | 0 | 0 | 5 | 13 | 10 | 0 | 1 | 5 | 9 | 8 |
| $\bar{2}$ | 3 | 0 | 3 | -1 | $\bar{4}$ | 8 | 0 | 5 | 3 | 1 | 0 | 5 | 6 | 2 | 0 | 2 | 5 | 10 | 8 |
| $\bar{3}$ | 3 | 0 | 8 | 8 | $\bar{5}$ | 8 | 0 | 4 | 2 | 2 | 0 | 5 | < 3 | 0 | 0 | 3 | 5 | 7 | 7 |
| $\bar{4}$ | 3 | 0 | 23 | 22 | 0 | 0 | 1 | 27 | 50 | $\bar{1}$ | 0 | 5 | 9 | 8 | 0 | $\bar{1}$ | 5 | 8 | 8 |
| $\bar{5}$ | 3 | 0 | 14 | 14 | 1 | 0 | 1 | 10 | 13 | $\bar{2}$ | 0 | 5 | 10 | 9 | 0 | $\bar{2}$ | 5 | 6 | 5 |
| $\bar{6}$ | 3 | 0 | 16 | 18 | 2 | 0 | 1 | 24 | 25 | $\bar{3}$ | 0 | 5 | 14 | 9 | 0 | $\bar{3}$ | 5 | 10 | 10 |
| $\bar{7}$ | 3 | 0 | 10 | 16 | 3 | 0 | 1 | 25 | 23 | $\bar{4}$ | 0 | 5 | 9 | 6 | 0 | $\bar{4}$ | 5 | 10 | 9 |
| $\bar{8}$ | 3 | 0 | < 4 | 3 | 4 | 0 | 1 | 23 | 24 | $\bar{5}$ | 0 | 5 | 7 | 8 | 0 | $\bar{5}$ | 5 | 12 | 12 |
| $\bar{9}$ | 3 | 0 | 8 | 7 | 5 | 0 | 1 | 21 | 23 | $\bar{6}$ | 0 | 5 | 7 | 6 | 0 | $\bar{6}$ | 5 | 7 | 7 |
| $\bar{10}$ | 3 | 0 | 6 | 6 | 6 | 0 | 1 | < 3 | -1 | 0 | 0 | 6 | 9 | 9 | 0 | $\bar{1}$ | 6 | 6 | 8 |
| 0 | 4 | 0 | 17 | 16 | 7 | 0 | 1 | < 3 | 2 | $\bar{1}$ | 0 | 6 | 8 | 8 | 0 | $\bar{2}$ | 6 | < 3 | 1 |
| 1 | 4 | 0 | 17 | 17 | 8 | 0 | 1 | 12 | 13 | $\bar{2}$ | 0 | 6 | 9 | 6 | 0 | $\bar{3}$ | 6 | < 3 | 2 |
| 2 | 4 | 0 | 10 | 9 | 9 | 0 | 1 | 6 | 8 | $\bar{3}$ | 0 | 6 | 6 | 6 | 0 | $\bar{4}$ | 6 | 10 | 9 |
| 3 | 4 | 0 | 6 | 6 | $\bar{1}$ | 0 | 1 | 16 | 25 | $\bar{4}$ | 0 | 6 | 6 | 2 |  |  |  |  |  |
| 4 | 4 | 0 | 5 | 4 | $\bar{2}$ | 0 | 1 | 31 | -34 | 0 | 1 | 1 | 13 | -11 |  |  |  |  |  |

be equal to the reliability index. The standard deviations in bond angles were estimated by the method of Darlow (1960).

## Description of the structure and discussion

### (*a*) *Molecular structure*

The intramolecular bond lengths and angles (Fig. 1 and Table 3) are normal within experimental error. As in the structures of nickel glycine dihydrate (Stosick, 1945), nickel di-$\alpha$-aminoisobutyrate tetrahydrate (Noguchi, 1962), copper proline dihydrate (Mathieson & Welsh, 1952), bis-($\beta$-aminobutyrato)-copper(II) dihydrate (Bryan, Poljak & Tomita, 1961) and copper $\beta$-alanine hexahydrate (Tomita, 1961), the two carboxylic oxygen atoms O(1), the two nitrogen atoms and the two water molecular oxygen atoms O(3) form an octahedron around the metal atom. In the case of copper compounds, however, the octahedra are very much distorted, with the water oxygen atoms at distances of about 2·5 Å and the nitrogen and carboxylic oxygen atoms at distances of about 2·0 Å from the copper atom; in the case of nickel compounds, the distortion from octahedral symmetry is very slight. The almost regular octahedral arrangement of ligands in the case of nickel compounds and the distorted octahedral arrangement in the case of copper compounds are in agreement with the conclusions of the theory of Orgel (1952), based on the Jahn–Teller effect (Orgel & Dunitz, 1957).

Table 3. *Intramolecular bond lengths and angles*

| Bond lengths | | Bond angles | |
|---|---|---|---|
| N–C(1) | 1·500 ± 0·040 Å | N–C(1)–C(2) | 109·6 ± 2·4° |
| C(1)–C(2) | 1·565 ± 0·043 | C(1)–C(2)–C(3) | 112·5 ± 2·5 |
| C(2)–C(3) | 1·545 ± 0·043 | C(2)–C(3)–O(1) | 125·9 ± 2·8 |
| C(3)–O(1) | 1·215 ± 0·038 | C(2)–C(3)–O(2) | 114·1 ± 2·5 |
| C(3)–O(2) | 1·279 ± 0·038 | O(1)–C(3)–O(2) | 122·7 ± 2·9 |
| Ni–N | 2·096 ± 0·026 | O(1)–Ni–N | 91·4 ± 1·0 |
| Ni–O(1) | 2·140 ± 0·023 | Ni–N–C(1) | 115·2 ± 1·9 |
| Ni–O(3) | 2·167 ± 0·023 | Ni–O(1)–C(3) | 123·2 ± 2·1 |

The line joining the water oxygen atoms O(3) and the nickel atom makes an angle of 88·2° with the plane containing the nickel atom, the two nitrogen atoms and the two carboxylic oxygens O(1). The sides of the octahedron around the nickel atom are: O(3)–N, 2·96 ± 0·04 Å and 3·07 ± 0·04 Å; O(3)–O(1), 3·03 ± 0·03 Å and 3·06 ± 0·03 Å; and N–O(1), 3·03 ± 0·04 Å and 2·96 ± 0·04 Å.

The mean plane through the atoms O(1), O(2), C(2) and C(3) can be represented by the equation

$$3{\cdot}564x' - 0{\cdot}588y' - 2{\cdot}969z' = 3{\cdot}341\ ,$$

where $x'$, $y'$ and $z'$ are the atomic coordinates (in Å) with reference to orthogonal axes $a$, $b'$ and $c'$, such that the $ab$ plane and the $ab'$ plane are the same. The normal distances of the individual atoms from the mean plane are 0·022 Å for O(1), O(2) and C(2), and −0·023 Å for C(3). The angle between this plane and the one containing the atoms C(1), C(2) and C(3)

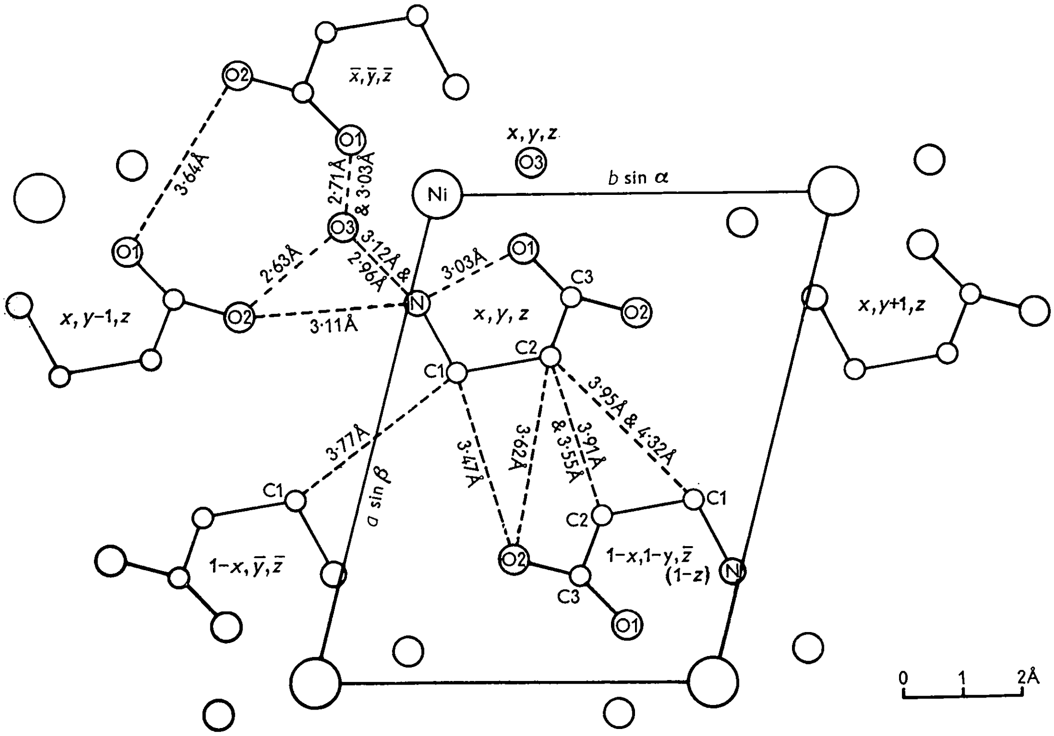

Fig. 2. Structure projected on (001).

is 30·3°, while the angle between the plane passing through C(1), C(2) and C(3), and the one containing the atoms N, C(1) and C(2) is 73·7° (70° in copper β-alanine hexahydrate; Tomita, 1961).

### (b) *Crystal structure*

The projection of the structure along the *c* axis is shown in Fig. 2. The nickel β-alanine dihydrate units are held together in a stable layer structure parallel to the (100) plane by the following bonds:

| | |
|---|---|
| O(1)($x, y, z$)–O(3)($x, y, z-1$) | 2·71 ± 0·03 Å |
| N ($x, y, z$)–O(3)($\bar{x}, \bar{y}, 1-z$) | 3·12 ± 0·04 Å |
| O(2)($x, y, z$)–O(3)($\bar{x}, 1-y, \bar{z}$) | 2·63 ± 0·03 Å |
| N ($x, y, z$)–O(2)($x, y-1, z$) | 3·11 ± 0·04 Å |

The hydrogen atoms of the water molecule make the two hydrogen bonds O(3)–O(1) and O(3)–O(2). If the N–H and N–C bonds about the nitrogen atom are assumed to be coplanar and to make angles of about 120° with each other, the possible hydrogen bonds with the nitrogen atom would also be expected to be roughly coplanar with the C–N bond and to make angles of the order of 120° with it. The angles between the C(1)–N bond and the contacts N–O(2) (3·11 Å), N–O(3) (3·12 Å) and N–O(3) (2·96 Å) are 103·3 ± 1·7°, 147·6 ± 1·9° and 100·6 ± 1·7° respectively; further the C(1)–N bond and the two N–O(3) contacts are coplanar within about 15° (Fig. 2). It seems therefore that either the two N–O(3) contacts are the possible hydrogen bonds or the contact N–O(2) is a possible hydrogen bond. The angles between the possible hydrogen bonds around the water oxygen atom O(3) are: 140·7 ± 1·2° between O(3)–O(1) (2·71 Å) and O(3)–O(2) (2·63 Å); 123·7 ± 1·1° between O(3)–O(1) (2·71 Å) and O(3)–N (2·96 Å); 60·7 ± 0·8° between O(3)–O(1) (2·71 Å) and O(3)–N (3·12 Å); 118·5 ± 1·1° between O(3)–O(2) (2·63 Å) and O(3)–N (3·12 Å); 67·3 ± 0·9° between O(3)–O(2) (2·63 Å) and O(3)–N (2·96 Å); and 108·4 ± 1·0° between O(3)–N (3·12 Å) and O(3)–N (2·96 Å).

The stacking of the layers normal to the (100) plane is governed by the van der Waals bonds of the type $CH_2$–$CH_2$ and $CH_2$–O, as shown in Fig. 2. It is thus clear that the crystal structure of nickel β-alanine dihydrate is similar to the structures of nickel glycine dihydrate (Stosick, 1945), bis-(β-aminobutyrato)copper(II) dihydrate (Bryan, Poljak & Tomita, 1961) and copper proline dihydrate (Mathieson & Welsh, 1952).

The *B* values of the atoms for the 0*kl* reflexions are in general smaller than those for the *hk*0 and *h*0*l* reflexions, thereby indicating, as expected, larger thermal vibration amplitudes normal to the layers of molecules.

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# Variation with Temperature of the Elastic Compliances of Potassium Iodide

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The thermo-elastic behaviour of a single crystal of potassium iodide has been investigated, from the boiling point of liquid oxygen to 300 °C. The composite piezoelectric oscillator method is the experimental technique employed. The compliances $S_{11}$ and $S_{44}$ increase with temperature, whereas the non-diagonal constant $S_{12}$ decreases with temperature.

## Introduction

The alkali halides constitute an important group among the cubic crystals. The physical properties, especially the elastic behaviour, of this group have been extensively studied, perhaps because of the simplicity of their structure. The effects of temperature on the elastic constants of potassium chloride and potassium bromide have been investigated by Durand (1936), Galt (1948), and Subrahmanyam (1958). In the case of potassium iodide the elastic constants at laboratory temperature were determined by