ment, de l'autre couche. Une attraction de type ionique peut donc intervenir dans les forces qui lient chaque couche de molécules à la voisine, bien que la distance Cl–N' = 3,50 Å soit supérieure à la somme des rayons de van der Waals. Des dispositions analogues ont d'ailleurs été déja signalées dans d'autres chlorhydrates d'amine: pipéridine (Rérat, 1960b) et pyridine (Rérat, 1962a) par exemple.

Entre les autres atomes appartenant à deux couches voisines on a trouvé des distances qui sont toutes supérieures à 3,6 Å. Finalement la cohésion entre couches semble être assurée principalement par les forces de van der Waals, ce qui s'accorde d'ailleurs avec l'observation, sur les cristaux, d'un plan de clivage très aisé perpendiculaire à l'axe d'allongement c.

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The Crystal and Molecular Structure of β-Alanine*

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β-Alanine, $NH_2CH_2CH_2COOH$, crystallized from aqueous solution, is orthorhombic, space group *Pbca* with eight molecules per unit cell of dimensions

$$a = 9 \cdot 865, \quad b = 13 \cdot 81, \quad c = 6 \cdot 07 \text{ Å}.$$

The structure was determined from the three Harker lines $P(U, \frac{1}{2}, 0)$, $P(0, V, \frac{1}{2})$ and $P(\frac{1}{2}, 0, W)$ and was refined with the help of general reflexions by the least-squares method.

The disposition of the hydrogen bonds around the nitrogen atom seems to indicate that the molecules in the crystal exist in the zwitterion form. The $N-H \cdots O$ hydrogen bonds tie the molecules into infinite double layers; each double layer is linked to the neighbouring double layers by van der Waals bonds.

Introduction

The structures of some metal complexes of β-alanine have recently been determined (Tomita, 1961; Jose, Pant & Biswas, 1964). In the present paper, the structure analysis of β-alanine is reported.

Experimental

Crystals were obtained from aqueous solution. They are orthorhombic and grow as plates parallel to the (100) face. The crystals show cleavage parallel to the (010) plane. The unit-cell dimensions are:

$$a = 9 \cdot 865, \quad b = 13 \cdot 81, \quad c = 6 \cdot 07 \text{ Å}.$$

The axial lengths were determined from high angle reflexions in zero layer Weissenberg photographs along the a and c axes. The cell dimensions reported by McCrone & Krc (1950) are:

$$a = 9 \cdot 86, \quad b = 13 \cdot 81, \quad c = 6 \cdot 09 \text{ Å}.$$

The observed density at 24 °C, measured by the flotation method, is 1·423 g.cm⁻³ and the calculated density for eight molecules of $NH_2CH_2CH_2COOH$ per unit cell is 1·431 g.cm⁻³. The observed density, measured by McCrone & Krc (1950) by the pycnometer method is 1·412 g.cm⁻³.

From the systematic absences, the space group is uniquely determined as *Pbca*. The linear absorption coefficient μ for Cu $K\alpha$ radiation is 11·5 cm⁻¹. The dimensions of the specimens used were roughly 0·7 mm along the c axis, 0·6 mm along the b axis and 0·3 mm along the a axis. The intensity data were obtained with Cu $K\alpha$ radiation and the multiple film technique from zero to fourth layer equi-inclination Weissenberg photographs along the c axis and from zero to sixth layer photographs along the a axis. 240 independent reflexions were observed out of possible 917 within the Cu $K\alpha$ limiting sphere. Intensities were measured visually and corrected for the Lp factor

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in the usual way. Intensities of the higher layer reflexions were generally measured from the extended ones and corrected for the effect of spot extension by the method of Phillips (1956). The harmonic mean of the intensities of the extended and contracted spots was taken for some reflexions for which the extension and contraction of spots was not much. Absorption was neglected.

Overall temperature factors for the $hk0$, $hk1$, $kh2$ and $0kl$ reflexions obtained by Wilson's method (1942) are 2·4, 1·8, 1·6 and 0·9 Å² respectively. A value of 1·2 Å² was used for the remaining reflexions. For reflexions of the type $0kl$ which are common with reflexions of the type $hk0$, $hk1$ $hk2$ etc. (e.g. $0k0$, $0k1$, $0k2$), a B value of 0·9 Å² only was used. The intensities of reflexions in different photographs were brought to the same scale with the help of common reflexions. The scale factors were improved in the later stages of refinement with the help of calculated structure factors. The structure factors were calculated with McWeeny's (1951) values of atomic scattering factors.

Determination and refinement of the structure

An attempt was first made to fix the trial structure with the help of (001) and (100) Patterson projections. A suitable trial structure, however, could not be postulated. An attempt to get the trial structure for the (001) projection with the help of statistical relations too did not succeed. The structure could ultimately be solved from the three Harker lines $P(U, \frac{1}{2}, 0)$, $P(0, V, \frac{1}{2})$ and $P(\frac{1}{2}, 0, W)$, shown in Fig. 1, 2 and 3 respectively. For a crystal with space group $Pbca$, peaks are expected at $(\frac{1}{2}-2x, \frac{1}{2}, 0)$ in the Harker line $P(U, \frac{1}{2}, 0)$ due to interaction between atoms related by b-glide, at $(0, \frac{1}{2}-2y, \frac{1}{2})$ in the $P(0, V, \frac{1}{2})$ line due to interaction between atoms related by c-glide and at $(\frac{1}{2}, 0, \frac{1}{2}-2z)$ in the $P(\frac{1}{2}, 0, W)$ line due to interaction between atoms related by a-glide. In the $P(0, V, \frac{1}{2})$ line (Fig. 2) there are two independent peaks at $V = 0·183$ and $0·322$ respectively. This suggests that the atoms in the molecule lie in two groups, the first group of atoms giving rise to the peak at 0·183 and the other group of atoms to the peak at 0·322. Owing to the presence of cleavage parallel to (010), it appeared likely that the hydrogen bonded molecules are arranged in layers parallel to (010). After some trial and with the help of a $\varrho(0, y, 0)$ line synthesis and difference synthesis, it was found that the stronger peak in the Harker line corresponds to the carboxyl and the amine group and the weaker peak corresponds to the two methylene groups.

There are four independent peaks A, B, C and D at $U = 0$, 0·230, 0·332 and 0·500 respectively in the $P(U, \frac{1}{2}, 0)$ line (Fig. 1). Assuming expected bond lengths and angles and with the help of approximate y parameters, it could be found after some trial and error that peak A corresponds to the atoms $C(1)$ (x, y, z and $\frac{1}{2}-x, \bar{y}, \frac{1}{2}+z$) and $N(x, y, z$ and $\frac{1}{2}-x, \bar{y}, \frac{1}{2}+z)$, B and

C correspond to $O(1)$ ($\bar{x}, \bar{y}, \bar{z}$) and $C(2)$ (x, y, z) respectively and D corresponds to $O(2)$ (x, y, z and $\bar{x}, \bar{y}, \bar{z}$) and $C(3)$ (x, y, z and $\bar{x}, \bar{y}, \bar{z}$) (Fig. 5). The approximate x and y parameters, obtained from $P(U, \frac{1}{2}, 0)$ and $P(0, V, \frac{1}{2})$ lines respectively were refined by the usual methods till R, on including all except high angle unobserved reflexions at half the minimum observable value, was 0·182. 040 appears to be subject to extinction and was left out of all calculations.
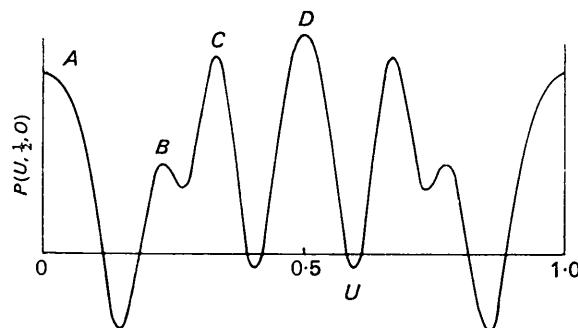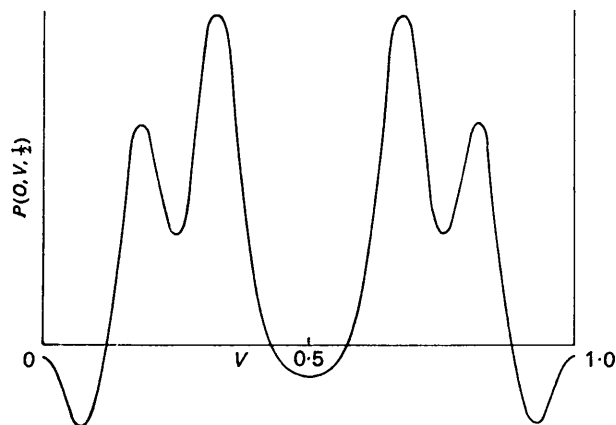

Fig. 1. $P(U, \frac{1}{2}, 0)$ line.
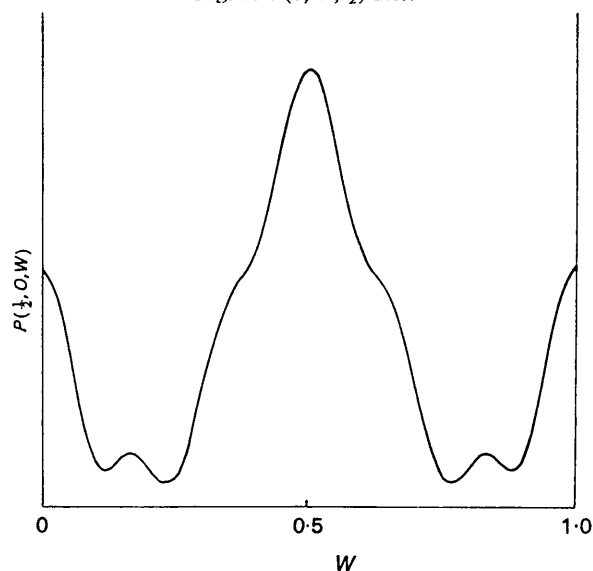

Fig. 2. $P(0, V, \frac{1}{2})$ line.

Fig. 3. $P(\frac{1}{2}, 0, W)$ line.

From the expected bond lengths and angles and the known x and y parameters, a model of the molecule in the (100) projection was made. The molecule was then shifted along the c axis till the two peaks at $W=0$ and 0.5 in the $P(\frac{1}{2}, 0, W)$ line, (Fig. 3) were explained. The z parameters thus obtained were refined with the help of $0kl$ reflexions till R, on including unobserved reflexions, was 0·187. 002 appears to be subject to extinction and was excluded from all calculations. As the atom O(2) ($z=0.2655\pm0.0009$, Table 1) lies close to the a-glide plane (x, y, $\frac{1}{4}$), it was not possible to distinguish with certainty between O(2) (x, y, z) and O(2) ($\frac{1}{2}+x$, y, $\frac{1}{2}-z$) from the (100) projection from bond length considerations. This point could be settled with the help of a few general reflexions.

Table 1. *Final atomic parameters*

	x/a	y/b	z/c
N	0.2955 ± 0.0006	0.0663 ± 0.0004	-0.0450 ± 0.0010
C(1)	0.2318 ± 0.0007	0.1599 ± 0.0005	0.0120 ± 0.0012
C(2)	0.0850 ± 0.0007	0.1601 ± 0.0005	-0.0796 ± 0.0012
C(3)	-0.0214 ± 0.0007	0.1107 ± 0.0005	0.0717 ± 0.0012
O(1)	-0.1393 ± 0.0005	0.0969 ± 0.0004	-0.0156 ± 0.0009
O(2)	0.0174 ± 0.0005	0.0851 ± 0.0004	0.2655 ± 0.0009

The atomic parameters obtained from the (100) and (001) projections were then used to calculate $F(hkl)$. R for 293 structure factors, including unobserved reflexions, was 0·177. A least-squares refinement was carried out after giving half weight to all ΔF values above 8 (thirteen of them). The maximum shift in atomic coordinates was about 0·03 Å and the value
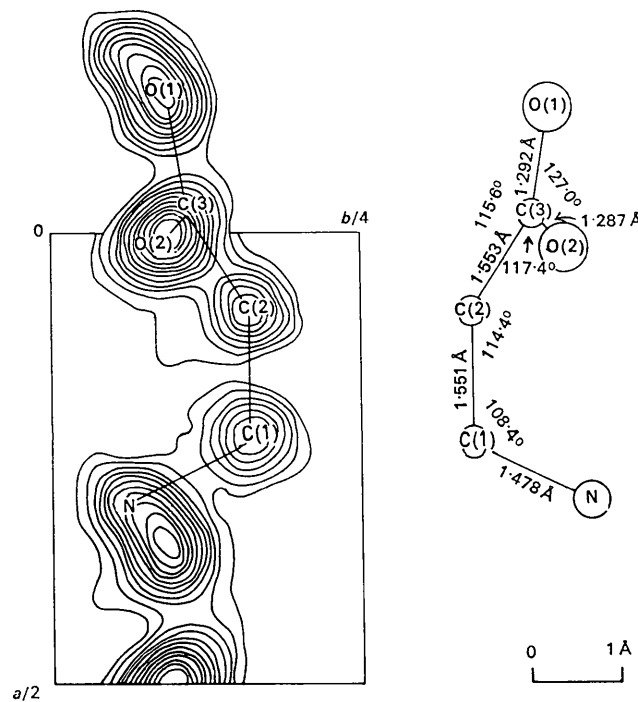
of R after refinement was 0·157. The agreement index, $\Sigma|\Delta F|/\Sigma|F|$ between 148 common F_o, obtained separately from the Weissenberg photographs along the a axis and from photographs along the c axis, is 0·166.

The (001) electron density projection (Fig. 4) was obtained with calculated signs and F_o values for all except 040 for which the final F_c were used. The final atomic parameters are listed in Table 1 and F_o and F_c in Table 2.

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

Molecular structure

The intramolecular bond lengths and angles are shown in Fig. 4 and listed in Table 3.

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

$$-0.290x+0.891y+0.348z-1.563=0,$$

where x, y, z are expressed in Å and referred to the axes of the unit cell. The normal distances of the individual atoms from the mean plane are $+0.013$ Å for C(3) and -0.004 Å for O(1), O(2) and C(2). The angle between this plane and the one containing atoms C(1), C(2) and C(3) is 9·3° (30·3° in nickel β-alanine dihydrate), while the angle between the plane passing through C(1), C(2), C(3) and the one containing atoms N, C(1), C(2) is 83·8° (73·7° in nickel β-alanine dihydrate and 70° in copper β-alanine hexahydrate).

Crystal structure

The projection of the structure along the c axis is shown in Fig. 5; the intermolecular distances are also indicated in the Figure. The nitrogen atom N (x, y, z) is immediately surrounded by four oxygen atoms O(1) ($\frac{1}{2}+x$, y, $-\frac{1}{2}-z$), O(2) ($\frac{1}{2}+x$, y, $\frac{1}{2}-z$), O(1) ($\bar{x}$, $\bar{y}$, $\bar{z}$) and O(2) ($\frac{1}{2}-x$, $\bar{y}$, $z-\frac{1}{2}$) at distances 2.78 ± 0.01, 2.78 ± 0.01, 2.76 ± 0.01 and 3.02 ± 0.01 Å respectively. The angles which the probable hydrogen bonds around the nitrogen atom make with the C(1)$-$N bond of the molecule and with each other are:

C(1)–N–O(1) ($\bar{x}$, $\bar{y}$, $\bar{z}$), $116.4\pm0.4°$;

C(1)–N–O(2) ($\frac{1}{2}+x$, y, $\frac{1}{2}-z$), $96.4\pm0.4°$;

C(1)–N–O(1) ($\frac{1}{2}+x$, y, $-\frac{1}{2}-z$), $101.0\pm0.4°$;

O(1) ($\frac{1}{2}+x$, y, $-\frac{1}{2}-z$) $-$N–O(2) ($\frac{1}{2}+x$, y, $\frac{1}{2}-z$),

$112.9\pm0.3°$;

O(1) ($\bar{x}$, $\bar{y}$, $\bar{z}$) $-$N–O(2) ($\frac{1}{2}+x$, y, $\frac{1}{2}-z$), $115.6\pm0.3°$;

O(1) ($\bar{x}$, $\bar{y}$, $\bar{z}$) $-$N–O(1) ($\frac{1}{2}+x$, y, $-\frac{1}{2}-z$),

$112.4\pm0.3°$;

Fig. 4. (001) electron density projection. Contours at intervals of 1 e.Å^{-2}, starting from 2 e.Å^{-2}.

Table 2. *Observed and calculated structure factors*

| h	k	l	|Fo|	F_c	h	k	l	|Fo|	F_c	h	k	l	|Fo|	F_c	h	k	l	|Fo|	F_c
2	0	0	17	24	1	3	1	48	-58	6	4	2	<10	6	9	0	4	13	-16
4	0	0	41	43	2	3	1	17	-15	7	4	2	<13	-6	2	1	4	13	13
6	0	0	18	20	3	3	1	19	16	1	5	2	16	19	3	1	4	<10	-11
8	0	0	18	18	4	3	1	16	-10	2	5	2	29	29	4	1	4	<12	-4
10	0	0	13	8	5	3	1	10	-7	3	5	2	14	15	5	1	4	24	-24
2	1	0	<8	6	0	4	1	38	-42	4	5	2	16	-10	6	1	4	18	-16
4	1	0	36	-30	1	4	1	25	24	6	5	2	21	20	0	2	4	25	23
6	1	0	17	-14	2	4	1	56	-56	7	5	2	14	14	2	2	4	11	11
8	1	0	18	17	3	4	1	34	35	8	5	2	17	-14	3	2	4	15	-16
0	2	0	62	56	4	4	1	22	-21	0	6	2	<12	9	5	2	4	<11	2
2	2	0	10	11	6	4	1	13	-9	2	6	2	25	32	6	2	4	12	10
4	2	0	9	12	1	5	1	29	-36	3	6	2	20	19	1	3	4	19	-19
6	2	0	31	31	2	5	1	15	15	4	6	2	36	41	2	3	4	21	19
8	2	0	<12	4	5	5	1	11	9	6	6	2	13	-12	3	3	4	<12	-13
2	3	0	59	63	7	5	1	37	31	7	6	2	14	-13	4	3	4	20	-19
4	3	0	37	-46	0	6	1	13	12	1	7	2	16	14	5	3	4	23	-28
6	3	0	9	-10	1	6	1	26	-25	2	7	2	33	36	6	3	4	19	-16
8	3	0	12	-1	2	6	1	<12	2	0	8	2	<15	3	0	4	4	38	-34
0	4	0	94	-154	4	6	1	15	11	2	8	2	26	30	2	4	4	<12	5
2	4	0	31	-33	1	7	1	17	15	2	9	2	24	-26	4	4	4	<12	-3
4	4	0	12	-15	2	7	1	18	16	0	10	2	<16	-9	3	5	4	12	9
6	4	0	17	-13	5	7	1	24	18	4	10	2	21	-25	4	5	4	15	-16
8	4	0	12	-18	7	7	1	33	-23	2	11	2	<14	8	0	6	4	34	-35
2	5	0	47	41	0	8	1	30	36	0	12	2	<17	7	2	6	4	19	-21
4	5	0	24	-23	1	8	1	35	-42	0	14	2	<16	-8	3	6	4	19	23
6	5	0	15	11	2	8	1	35	33	1	1	3	25	28	6	6	4	16	-18
8	5	0	31	-29	3	8	1	20	-18	4	1	3	39	40	1	7	4	21	16
0	6	0	60	-69	4	8	1	19	18	5	1	3	11	-7	2	7	4	11	-10
2	6	0	34	-31	1	9	1	19	16	7	1	3	19	20	3	7	4	17	20
4	6	0	10	-11	5	9	1	13	15	8	1	3	19	16	4	7	4	18	14
6	6	0	54	-51	0	10	1	<16	8	0	2	3	45	52	0	8	4	<17	-14
8	6	0	12	-11	1	10	1	23	20	1	2	3	<11	-7	4	8	4	12	-12
2	7	0	42	-40	0	12	1	<17	-11	2	2	3	8	8	0	10	4	<17	11
4	7	0	<10	2	1	12	1	25	27	3	2	3	31	34	4	10	4	14	-14
6	7	0	<13	10	0	14	1	<17	-7	4	2	3	<11	-6	0	12	4	25	23
0	8	0	23	-26	1	15	1	21	-16	5	2	3	27	-33	3	1	5	19	-21
2	8	0	22	18	0	0	2	64	108	9	2	3	12	11	4	1	5	18	15
4	8	0	<12	-10	1	0	2	31	29	1	3	3	17	-13	5	1	5	<9	-7
6	8	0	<12	3	2	0	2	66	-80	2	3	3	17	-19	6	1	5	13	-9
8	8	0	<6	6	3	0	2	22	18	3	3	3	12	14	0	2	5	<16	-2
10	8	0	10	-8	4	0	2	32	-32	4	3	3	16	-14	2	2	5	24	-24
2	9	0	27	-22	5	0	2	21	22	5	3	3	14	-9	3	2	5	22	23
4	9	0	18	17	6	0	2	20	-18	0	4	3	29	35	4	2	5	24	-26
6	9	0	<12	8	7	0	2	14	-6	1	4	3	13	14	5	2	5	15	-15
0	10	0	16	17	8	0	2	<13	2	2	4	3	9	-8	6	2	5	15	-11
2	10	0	24	27	2	1	2	27	22	3	4	3	11	5	3	3	5	14	10
4	10	0	<12	-5	3	1	2	<9	-6	4	4	3	22	23	5	3	5	9	-8
6	10	0	28	26	4	1	2	<9	-4	6	4	3	21	18	0	4	5	<16	2
8	10	0	16	12	5	1	2	27	-22	8	4	3	16	5	2	4	5	30	-31
2	11	0	14	15	6	1	2	<10	-1	1	5	3	21	-25	3	5	5	22	20
4	11	0	19	18	7	1	2	<13	-4	4	5	3	16	-19	5	5	5	17	16
0	12	0	35	46	8	1	2	22	23	5	5	3	10	7	4	6	5	12	13
6	13	0	12	-14	0	2	2	<8	-1	6	5	3	15	16	5	7	5	11	13
8	13	0	12	11	2	2	2	29	-24	7	5	3	23	-24	2	8	5	21	22
0	14	0	<17	-1	3	2	2	21	-16	0	6	3	20	16	5	9	5	11	-14
0	16	0	21	-25	4	2	2	24	-23	1	6	3	14	-13	0	0	6	<17	-12
1	1	1	43	59	5	2	2	<9	4	4	6	3	16	16	2	0	6	35	-33
2	1	1	10	-9	6	2	2	<10	6	2	7	3	15	15	4	0	6	19	-14
3	1	1	<14	4	7	2	2	<13	7	5	7	3	18	11	5	0	6	9	10
5	1	1	24	-25	1	3	2	16	-8	0	8	3	<15	-10	2	1	6	14	11
6	1	1	15	-15	2	3	2	53	62	1	8	3	21	-26	6	1	6	9	-10
7	1	1	29	25	4	3	2	10	-10	0	10	3	42	-36	0	2	6	<17	-4
8	1	1	<22	-6	5	3	2	22	-18	0	12	3	21	-17	2	2	6	<8	-1
0	2	1	31	-38	6	3	2	13	14	1	12	3	19	19	4	2	6	15	-15
1	2	1	36	-37	7	3	2	<13	7	0	14	3	22	18	2	3	6	12	10
2	2	1	47	-57	8	3	2	17	20	0	0	4	61	66	5	3	6	10	-8
3	2	1	56	52	10	3	2	20	21	1	0	4	20	13	6	3	6	9	-8
4	2	1	54	-48	0	4	2	43	-53	2	0	4	<9	-9	0	4	6	<17	7
5	2	1	36	-41	1	4	2	<9	-4	3	0	4	<10	5	2	4	6	19	22
6	2	1	30	-28	2	4	2	23	24	4	0	4	14	14	4	4	6	13	10
7	2	1	<21	16	3	4	2	17	-15	5	0	4	18	14	4	6	6	23	28
8	2	1	<23	-14	4	4	2	20	21	6	0	4	17	15	4	7	6	12	11
9	2	1	41	30	5	4	2	12	-14	7	0	4	<12	-9	0	2	7	21	16
										8	0	4	15	20	0	4	7	24	28
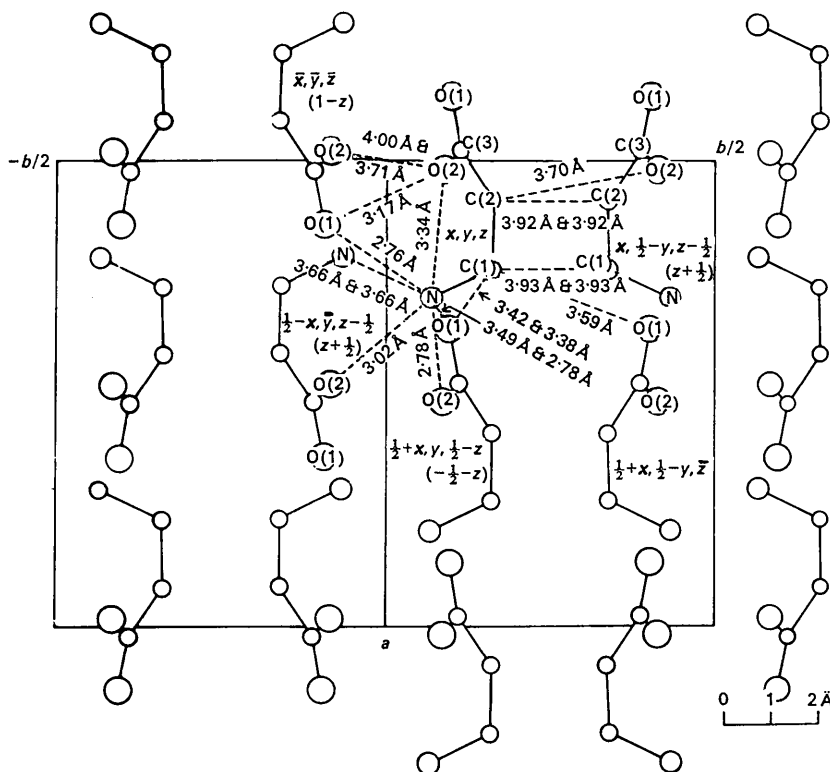
Fig. 5. Structure projected on (001). Interatomic distances in Å.

Table 3. *Intramolecular bond lengths and angles*

	Bond lengths		Bond angles
N–C(1)	1·478 ± 0·010 Å	N–C(1)–C(2)	108·4 ± 0·6°
C(1)–C(2)	1·551 ± 0·010	C(1)–C(2)–C(3)	114·4 ± 0·6
C(2)–C(3)	1·553 ± 0·010	C(2)–C(3)–O(1)	115·6 ± 0·6
C(3)–O(1)	1·292 ± 0·009	C(2)–C(3)–O(2)	117·4 ± 0·6
C(3)–O(2)	1·287 ± 0·009	O(1)–C(3)–O(2)	127·0 ± 0·7

O(2) ($\frac{1}{2}-x$, $\bar{y}$, $z-\frac{1}{2}$) – N–C(1), 162·3 ± 0·5°;

O(2) ($\frac{1}{2}-x$, $\bar{y}$, $z-\frac{1}{2}$) – N–O(1) ($\bar{x}$, $\bar{y}$, $\bar{z}$), 80·0 ± 0·2°;

O(2) ($\frac{1}{2}-x$, $\bar{y}$, $z-\frac{1}{2}$) – N–O(2) ($\frac{1}{2}+x$, y, $\frac{1}{2}-z$),

79·4 ± 0·2°; and

O(2) ($\frac{1}{2}-x$, $\bar{y}$, $\bar{z}-\frac{1}{2}$) – N–O(1) ($\frac{1}{2}+x$, y, $-\frac{1}{2}-z$),

66·3 ± 0·2° .

The angles between N–O(2) ($\frac{1}{2}-x$, $\bar{y}$, $z-\frac{1}{2}$) and the other probable hydrogen bonds as well as the C(1)–N bond depart widely from the tetrahedral value (109·5°), whereas the other angles are all close to it. This indicates that there are three strong hydrogen bonds of lengths 2·78 ± 0·01, 2·78 ± 0·01 and 2·76 ± 0·01 Å around the nitrogen atom. The situation in β-alanine is thus different from that in α-glycine (Albrecht & Corey, 1939; Marsh, 1958) and in β-glycine (Iitaka, 1960); in these crystals there are two strong hydrogen bonds and two weak bonds (probably hydrogen bonds) around the nitrogen atom. The nearly tetrahedral arrangement of hydrogen bonds around the nitrogen atom also implies that β-alanine, like most of the amino acids, exists in the zwitterion form.

The β-alanine molecules are held together in a stable layer structure parallel to (010) by the hydrogen bonds NH $\cdots$ O(1) ($\frac{1}{2}+x$, y, $-\frac{1}{2}-z$) and NH $\cdots$ O(2) ($\frac{1}{2}+x$, y, $\frac{1}{2}-z$). Each layer is linked with the neighbouring layers by the hydrogen bond NH $\cdots$ O(1) ($\bar{x}$, $\bar{y}$, $\bar{z}$) on one side and by van der Waals bonds on the other. The arrangement of the hydrogen bonded layers of molecules is thus similar to that in the case of α-glycine (Albrecht & Corey, 1939).

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