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The Crystal and Molecular Structure of γ-Hydroxy-β-amino butyric Acid

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Abstract □ The crystal structure of γ-hydroxy-β-aminobutyric acid was determined by *MULTAN* system with X-ray intensity data on a diffractometer and refined by the least-squares method to an R-value 0.034 for 711 reflections. The crystals were orthorhombic, space group $P2_12_12_1$, Z=4, with a=10.220, b=8.257 and c=6.556Å. The molecule takes the zwitterionic form and skeletal conformation is trans-trans form. The molecules are held together by intra-and intermolecular NH---O and OH---O hydrogen bonds.

Keywords □ X-ray diffraction, γ-Hydroxy-β-aminobutyric acid, γ-amino-β-hydroxy butyric acid, GABA, GABOB, *MULTAN* system, Zwitterion, γ-Guanidino-β-hydroxy propane sulfonic acid, Taurine, Homotaurine, γ-Guanidinopropane sulfonic acid, Trans-trans, Hydrogen bonds.

γ-hydroxy-β-amino butyric acid (GOBAB) is a compound that was interchanged the radicals of hydroxyl and amino group in γ-amino-β-hydroxy butyric acid (GABOB)[1] which is a chemical transmitter in the central nervous system.

Author has been investigating systematically the molecular structures of related compounds of γ-amino butyric acid (GABA)[2], GABOB and other derivatives substituted with, such as guanidyl, sulfonyl and hydroxyl groups.

This paper presents the crystal and molecular structure of titled compound and some structural comparisons between related compounds.

EXPERIMENTAL METHODS

The compound was recrystallized from aqueous solution as colorless, transparent crystals.

Crystallographic Measurement

The space group was determined from rotation and Weissenberg photographs, and the lattice constants were obtained from precise measurement on a diffractometer with MoKα radiations. Density was measured by the flotation method in a mixture of chloroform and benzene. The crystal data are listed in Table I.

Three-dimensional intensity data were collected on a computer-controlled four circle diffractometer(Rigaku Denki Co. Ltd.) with Zr-filtered MoKα radiations. A total of 711 refle-

Table I: Crystal data of γ-hydroxy-β-amino butyric acid.

Molecular formula; $C_4H_9O_3N$	Mol. wt.; 119.12
colorless transparent	orthorhombic
a=10.220(6)Å	b=8.257(2)Å
c=6.556(8)Å	
Volume of unit cell	553.31Å^3
Density (by flotation)	1.42g/cm^3
Density (calculated)	1.43g/cm^3
Z=4	F(000)=256
Absent spectra;	h00 when h=2n+1
	0k0 when k=2n+1
	001 when l=2n+1
Space group; $P2_12_12_1$	

Table II: Observed and calculated structure factors of GOBAB.

H	K	L	Fo	Fc
0	2	0	9	9
0	4	0	10	10
0	6	0	19	19
0	8	0	8	8
1	1	0	10	11
1	2	0	17	17
1	3	0	34	34
1	4	0	15	15
1	5	0	10	10
1	6	0	2	2
1	7	0	4	4
2	0	0	30	30
2	1	0	29	30
2	2	0	15	15
2	3	0	20	20
2	4	0	27	26
2	5	0	2	2
2	6	0	8	8
2	7	0	28	28
2	8	0	3	3
3	1	0	7	7
3	2	0	3	3
3	3	0	15	15
3	4	0	18	18
3	6	0	2	2
3	7	0	11	10
3	8	0	3	2
3	9	0	2	2
4	0	0	41	41
4	1	0	18	17
4	2	0	16	15
4	3	0	45	44
4	4	0	6	6
4	5	0	8	8
4	6	0	3	3
4	7	0	2	2
5	1	0	11	12
5	2	0	17	16
5	3	0	5	5
5	5	0	8	8
5	6	0	13	13
5	7	0	4	4
5	8	0	2	0
6	0	0	8	8
6	1	0	4	3
6	2	0	7	7
6	3	0	6	6
6	4	0	24	24
6	7	0	3	4
6	8	0	6	6
7	1	0	2	2
7	2	0	14	14
7	3	0	6	6
7	4	0	5	6
7	6	0	11	11
7	7	0	6	6
8	1	0	8	8
8	2	0	7	7
8	3	0	22	23
8	4	0	4	4
8	6	0	2	0
8	7	0	3	3
9	1	0	2	1
9	2	0	3	2
9	3	0	4	4
9	4	0	11	11
9	7	0	3	3
10	0	0	8	8
10	1	0	4	4
10	3	0	2	2
10	4	0	9	8
10	5	0	3	3
10	6	0	6	5
10	7	0	7	6
11	1	0	3	3
11	3	0	5	5
11	4	0	3	3
11	5	0	2	2
0	1	1	11	12
0	2	1	21	22
0	3	1	34	34
0	4	1	16	16
0	5	1	12	13
0	6	1	16	16
0	7	1	30	31
1	0	1	6	5
1	1	1	23	23
1	2	1	16	17
1	3	1	26	26
1	4	1	13	13
1	5	1	4	4
1	6	1	1	2
1	7	1	14	14
1	8	1	2	2
1	9	1	4	4
2	0	1	99	102
2	1	1	15	15
2	2	1	8	8
2	3	1	46	46
2	4	1	9	8
2	5	1	1	2
2	6	1	15	16
2	7	1	5	5
2	8	1	3	3
2	9	1	5	5
3	0	1	43	42
3	1	1	23	23
3	2	1	4	3
3	3	1	17	16
3	4	1	13	13
3	5	1	12	12
3	6	1	6	6
3	7	1	7	6
3	8	1	4	5
4	0	1	8	9
4	1	1	13	12
4	2	1	13	14
4	3	1	17	17
4	4	1	22	21
4	5	1	10	10
4	6	1	9	9
4	7	1	9	10
4	9	1	3	3
5	0	1	16	15
5	1	1	19	19
5	2	1	16	16
5	3	1	8	8
5	5	1	3	3
5	6	1	1	1
5	7	1	7	8
5	8	1	2	2
5	9	1	3	3
6	0	1	9	9
6	1	1	11	11
6	3	1	16	16
6	4	1	5	5
6	5	1	1	2
6	6	1	4	4
6	8	1	4	4
7	0	1	14	14
7	1	1	14	13
7	2	1	6	7
7	3	1	8	8
7	4	1	5	5
7	5	1	5	5
7	6	1	2	2
7	7	1	5	5
7	9	1	4	3
8	0	1	3	3
8	1	1	2	2
8	3	1	11	12
8	4	1	13	13
8	5	1	7	7
8	6	1	2	2
9	0	1	8	8
9	1	1	4	3
9	2	1	4	3
9	3	1	2	4
9	4	1	4	3
9	5	1	4	3
9	6	1	2	2
9	7	1	5	5
10	0	1	8	9
10	3	1	13	13
10	5	1	3	3
10	7	1	3	3
11	1	1	4	4
11	2	1	2	2
11	3	1	4	4
11	4	1	4	4
0	0	2	54	54
0	1	2	21	21
0	2	2	47	47
0	3	2	9	9
0	4	2	10	9
0	5	2	3	3
0	6	2	13	13
0	7	2	3	3
0	8	2	2	3
0	9	2	5	5
1	0	2	49	48
1	1	2	19	19
1	2	2	17	17
1	3	2	13	12
1	4	2	16	16
1	5	2	5	4
1	6	2	4	4
1	7	2	7	7
1	8	2	8	9
1	9	2	3	3
2	0	2	28	28
2	1	2	11	11
2	2	2	28	28
2	3	2	16	16
2	4	2	9	9
2	5	2	9	9
2	6	2	14	14
2	7	2	9	10
2	8	2	4	4
2	9	2	2	2
3	0	2	2	1
3	1	2	16	16
3	2	2	9	9
3	3	2	14	13
3	4	2	6	6
3	5	2	9	9
3	6	2	5	5
3	7	2	13	13
3	8	2	3	3
3	9	2	2	2
4	0	2	5	5
4	1	2	2	2
4	2	2	8	8
4	3	2	11	11
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4	7	2	5	4
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5	5	2	9	8
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5	8	2	5	5
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6	4	2	6	7
6	5	2	5	6
6	6	2	2	2
6	7	2	4	4
6	8	2	3	3
7	0	2	10	10
7	2	2	4	3
7	3	2	13	13
7	4	2	4	4
7	5	2	4	4
7	6	2	4	4
7	7	2	3	3
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8	2	2	6	5
8	3	2	5	5
8	4	2	5	3
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8	7	2	4	3
9	0	2	3	2
9	1	2	2	2
9	2	2	4	3
9	3	2	8	8
9	5	2	5	5
9	6	2	5	5
10	0	2	7	7
10	1	2	2	2
10	2	2	2	2
10	3	2	4	4
10	4	2	5	4
10	6	2	4	3
11	0	2	5	4
11	1	2	4	4
11	2	2	3	3
0	1	3	1	0
0	2	3	5	6
0	3	3	25	25
0	4	3	7	7
0	5	3	16	16
0	6	3	5	4
0	7	3	3	3
0	9	3	2	2
1	0	3	27	27
1	1	3	13	13
1	2	3	13	13
1	3	3	9	9
1	4	3	6	6
1	5	3	11	11
1	6	3	8	8
1	7	3	9	9
1	8	3	7	7
1	9	3	4	4
2	0	3	3	3
2	1	3	20	19
2	2	3	17	17
2	3	3	12	12
2	4	3	10	10
2	5	3	11	11
2	6	3	5	5
2	7	3	10	9
2	8	3	4	4
3	0	3	28	26
3	1	3	24	24
3	2	3	5	4
3	3	3	14	14
3	4	3	12	12
3	5	3	7	7
3	6	3	7	7
3	7	3	5	6
3	8	3	3	3
3	9	3	3	3
4	0	3	20	20
4	1	3	7	7
4	2	3	11	11
4	3	3	5	5
4	4	3	12	12
4	5	3	3	4
4	6	3	5	5
4	7	3	4	4
4	8	3	2	2
5	0	3	8	8
5	1	3	12	12
5	3	3	10	10
5	4	3	12	13
5	5	3	3	3
5	6	3	6	6
5	7	3	7	7
5	8	3	2	2
6	1	3	14	15
6	2	3	7	7
6	3	3	7	6
6	4	3	8	9
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6	7	3	8	8
6	8	3	4	7
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7	2	3	3	3
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7	4	3	8	8
7	5	3	2	3
7	6	3	4	3
7	7	3	3	4
8	0	3	9	8
8	1	3	6	6
8	3	3	4	4
8	4	3	3	2
8	5	3	6	5
8	6	3	3	3
8	7	3	8	8
9	0	3	5	5
9	1	3	6	6
9	3	3	5	6
9	4	3	6	6
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10	4	3	3	3
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11	4	3	2	1
0	0	4	12	12
0	2	4	7	8
0	3	4	4	4
0	4	4	16	16
0	5	4	8	8
0	6	4	6	5
0	7	4	3	3
1	0	4	13	13
1	1	4	23	23
1	2	4	2	1
1	3	4	6	6
1	4	4	6	6
1	5	4	6	6
1	6	4	10	10
1	7	4	4	3
2	0	4	25	26
2	1	4	12	12
2	2	4	6	6
2	3	4	15	15
2	4	4	16	17
2	5	4	3	3
2	6	4	2	2
2	7	4	3	3
3	0	4	13	13
3	1	4	10	9
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3	4	4	6	6
3	5	4	3	4
3	6	4	10	10
3	7	4	3	3
4	0	4	9	9
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4	2	4	8	8
4	3	4	6	6
4	4	4	8	7
4	5	4	3	3
4	6	4	2	1
4	7	4	11	11
4	8	4	8	8
5	1	4	5	5
5	2	4	11	11
5	3	4	4	4
5	4	4	12	12
5	5	4	4	5
5	6	4	7	6
5	7	4	4	4
5	8	4	5	5
6	0	4	4	4
6	1	4	6	6
6	2	4	4	3
6	3	4	5	5
6	4	4	7	7
6	5	4	4	4
6	6	4	2	2
6	7	4	2	3
7	0	4	6	6
7	1	4	2	3
7	2	4	3	3
7	3	4	3	3
7	4	4	3	3
7	5	4	4	4
7	6	4	4	4
7	7	4	3	3
8	0	4	5	5
8	1	4	4	4
8	2	4	3	3
8	3	4	3	3
8	4	4	3	3
8	5	4	3	3
8	6	4	3	3
8	7	4	3	3
9	0	4	3	3
9	1	4	3	3
9	2	4	3	3
9	3	4	3	3
9	4	4	3	3
9	5	4	3	3
9	6	4	3	3
9	7	4	3	3
10	0	4	3	3
10	1	4	3	3
10	2	4	3	3
10	3	4	3	3
10	4	4	3	3
10	5	4	3	3
10	6	4	3	3
10	7	4	3	3
11	0	4	3	3
11	1	4	3	3
11	2	4	3	3
11	3	4	3	3
11	4	4	3	3
11	5	4	3	3
11	6	4	3	3
11	7	4	3	3

ctions limited within $\sin\theta/\lambda$ 0.55Å^{-1} were scanned by $\omega-2\theta$ techniques at a scan speed of 4° per minute. All the reflections were recorded and corrected for usual Lorentz and polarization effects, but no absorption correction being made.

Structure Determination and Refinement

An approximate scale and the over-all temperature factor were calculated by Wilson's method, but this calculation indicated that this compound is noncentrosymmetric and can not be applied to symbolic addition method to solve this structure. In this step, author used the *MULTAN* system[3] and all of the non-hydrogen atoms were revealed. Continuation of successive Fourier syntheses with overall isotropic temperature factors reduced the R-factor to 0.18.

Refinement was carried out for all reflections by the block-diagonal least-squares procedure with unit weight. The R-factor was reduced to 0.16 with isotropic temperature factors for all non-hydrogen atoms and decreased further with anisotropic temperature factors to 0.08. In this state, a difference Fourier synthesis revealed the locations of all the 9 hydrogen atoms. They were included in the final least-squares cycles with isotropic temperature factors. The final R-value was 0.034. The observed and calculated structure factors are listed in Table II.

Calculations were carried out on NEAC 2200-700 computer, Osaka University, Osaka, Japan, and IBM 370, Seoul National University, Seoul, Korea. The atomic scattering factors were taken from the "International Tables for X-Ray Crystallography."[4]

Table III: Final positional and thermal parameters (Estimated standard deviations in parentheses) Anisotropic temperature factors are expressed in the form of exp$[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)]$

Atom	X	Y	Z
C1	0.3931(4)	0.4424(5)	0.5791(6)
C2	0.3327(5)	0.6073(5)	0.6240(8)
C3	0.4049(5)	0.7482(5)	0.5261(7)
C4	0.3395(5)	0.9083(5)	0.5681(7)
N	0.4117(4)	0.7197(5)	0.3001(6)
O1	0.3332(3)	0.3199(3)	0.6433(5)
O2	0.4974(3)	0.4385(3)	0.4812(5)
O3	0.4190(4)	1.0324(4)	0.4831(6)

Atom	U_{11}	U_{22}	U_{33}
C1	0.0417(23)	0.0288(20)	0.0256(27)
C2	0.0407(24)	0.0261(18)	0.0311(28)
C3	0.0314(22)	0.0286(19)	0.0301(26)
C4	0.0429(23)	0.0269(21)	0.0346(30)
N	0.0373(21)	0.0264(18)	0.0249(22)
O1	0.0458(18)	0.0267(15)	0.0530(23)
O2	0.0438(16)	0.0317(14)	0.0448(20)
O3	0.0716(24)	0.0216(16)	0.0580(25)

Atom	U_{12}	U_{13}	U_{23}
C1	−0.0010(19)	−0.0039(21)	−0.0008(18)
C2	0.0028(19)	0.0077(23)	0.0002(20)
C3	0.0025(16)	−0.0042(22)	−0.0021(19)
C4	0.0015(19)	0.0099(24)	−0.0057(21)
N	−0.0006(16)	0.0050(19)	0.0020(17)
O1	−0.0029(15)	0.0092(18)	0.0028(16)
O2	0.0043(14)	0.0123(16)	−0.0001(15)
O3	−0.0021(16)	0.0218(22)	−0.0034(18)

RESULTS AND DISCUSSION

The final atomic parameters are given in Table III and IV, together with their estimated standard deviations. The difference Fourier map is shown in Fig. 1. As shown in Fig. 1, one hydrogen atom of carboxyl group is transfered to the amino group. Thus, the molecule occurs in the form of zwitterionic, $HOCH_2CH(NH_3^+)$

Table IV: Fractional coordinates of hydrogen atoms.

Atom	X	Y	Z	U
C2H1	0.238	0.607	0.597	0.04
C2H2	0.335	0.621	0.775	0.03
C3H1	0.509	0.750	0.574	0.04
C4H1	0.239	0.907	0.509	0.04
C4H2	0.329	0.921	0.721	0.04
NH1	0.325	0.705	0.235	0.06
NH2	0.459	0.630	0.265	0.04
NH3	0.442	0.803	0.229	0.02
O3H1	0.396	1.117	0.528	0.03

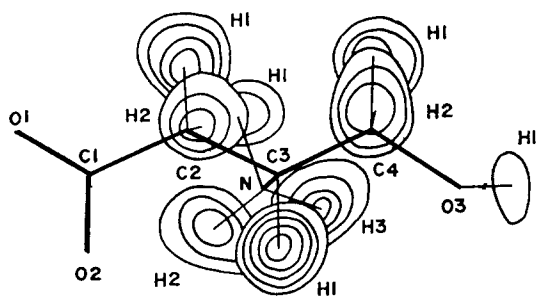

Fig. 1: Difference Fourier map of GOBAB. Contours are drawn at intervals of 0.1 e.Å^{-3}, starting with the contour of 0.2 e.Å^{-3}.

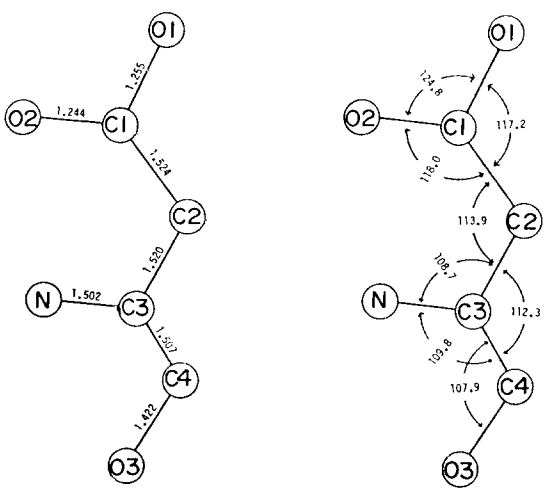

Fig. 2: Bond lengths (A) and angles (°) of GOBAB.

CH_2COO^-, as in the cases of related compounds.

Bond Distances and Angles

The interatomic distances and angles are listed in Fig. 2, and Table V, together with their estimated standard deviations. These values are reasonable compared with those of other related compounds such as GGBOPSA[5], GGPSA[6], taurine[7,8], homotaurine[9], GABOPSA[10], GABA and GABOB.

The C-H, N-H and O-H distances are within the ranges of 0.98~1.12Å, 0.89~0.99Å, and 0.79A, respectively. The distances of C-N and C-O (of hydroxyl group) have almost same values to those of corresponding bonds in GABOB.

Conformation

As shown in Fig. 3, the skeletal conformation of this molecule is trans-trans form, as found in GABOB, GABOPSA, GGBOPSA and homotaurine. However, the corresponding values of GABOB are 173.7° and 168.8°, respectively. This fully extended structure can be seen in the cases of GABOPSA and homotaurine.

Crystal Structure

Distances and angles of hydrogen bonds are listed in Table VI. All the feasible hydrogen atoms in the molecule are utilized to form intra- and intermolecular hydrogen bonds, in which two hydrogen atoms (NH2 and NH3) on the amino group take part in bifurcated hydrogen

Table V: Bond distances(Å) and angles(°).

C1-C2	1.524(6)*	∠O1-C1-O2	124.8(4)
C2-C3	1.520(6)	∠O1-C1-C2	117.2(3)
C3-C4	1.507(6)	∠O2-C1-C2	118.0(4)
C1-O1	1.255(4)	∠C1-C2-C3	113.9(4)
C1-O2	1.244(5)	∠C2-C3-C4	112.3(4)
C3-N	1.502(6)	∠C2-C3-N	108.7(4)
C4-O3	1.422(5)	∠C4-C3-N	109.8(4)
		∠C3-C4-O3	107.9(3)

* Estimated standard deviations are in parentheses

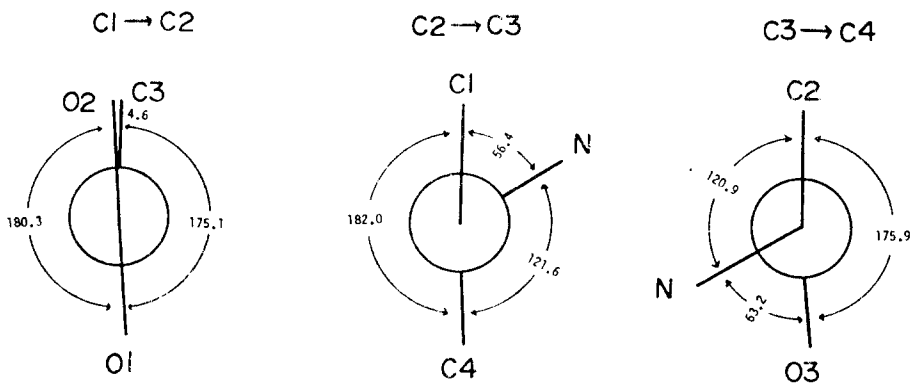

Fig. 3: Newman projection of atoms around three bonds.

bonds. Intramolecular hydrogen bonds are N-NH2---O2 and N-NH3---O3. Thus, the molecules are held together by three-dimensional network of intra- and intermolecular OH---O and NH---O hydrogen bonds, as shown in Fig. 4.

The intermolecular contacts between adjacent molecules are in normal van der Waals distances.

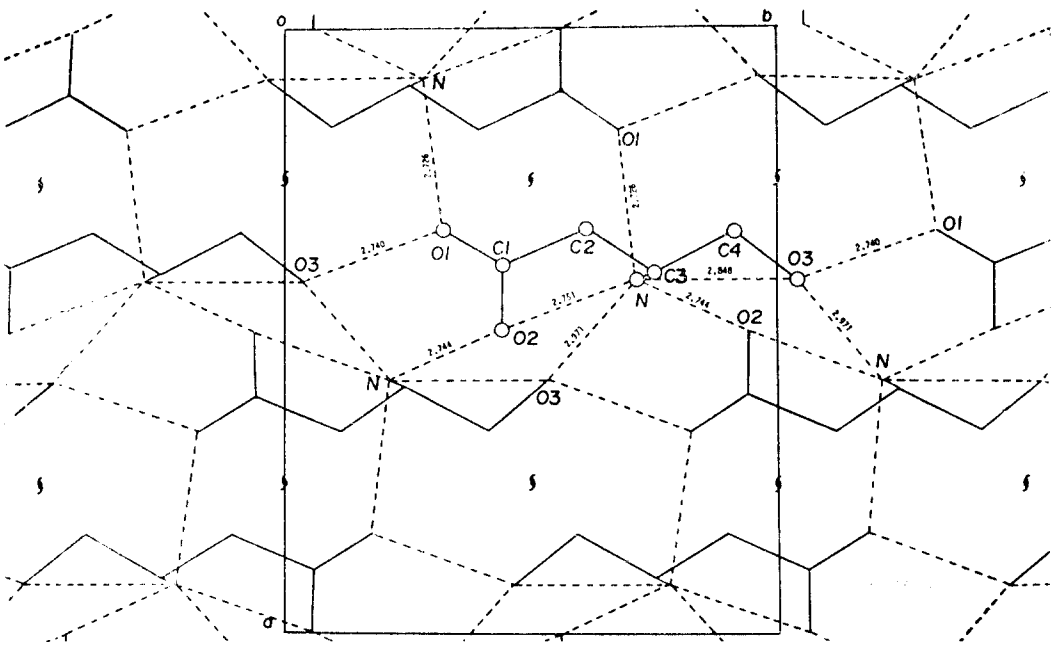

Fig. 4: The crystal structure projected along *c*-axis.

Table VI: Hydrogen Bond Lengths(Å) and Angles(°)

Bond lengths		Bond angles	
N-(NH2)---O2(Ⅰ)	2.751[a]	C3-N-O2(Ⅰ)	73.8[a]
N-(NH2)---O3(Ⅱ)	2.971[a]	C3-N-O3(Ⅱ)	72.6[a]
N-(NH3)---O2(Ⅲ)	2.744[b]	C3-N-O2(Ⅲ)	125.1[b]
N-(NH3)---O3(Ⅰ)	2.848[b]	C3-N-O3(Ⅰ)	56.2[b]
N-(NH1)---O1(Ⅳ)	2.726	C3-N-O1(Ⅳ)	110.4
O3-(O3H1)---O1(Ⅴ)	2.740	C4-O3-O1(Ⅴ)	106.9

(Ⅰ) (X, Y, Z)
(Ⅱ) $(1-X, -0.5+Y, 0.5-Z)$
(Ⅲ) $(1-X, 0.5+Y, 0.5-Z)$
(Ⅳ) $(0.5-X, 1-Y, -0.5+Z)$
(Ⅴ) $(X, 1+Y, Z)$
a), b) Bifurcated hydrogen bonds

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