Crystal and Molecular Structure of ω-Amino Acids, ω-Amino Sulfonic Acids and Their Derivatives. II. The Crystal and Molecular Structure of α-Form of 3-Aminopropane Sulfonic Acid, Homotaurine

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From ethanol aqueous solution, two forms of crystals of 3-aminopropane sulfonic acid (homotaurine) have been obtained in different crystal systems. The α-form is orthorhombic, space group $Pmn2_1$, with two molecules in a unit cell of the dimensions; $a=7.059$, $b=5.492$ and $c=7.428$ Å. The X-ray structure analysis was carried out by the application of usual heavy atom method and refined by three dimensional least-squares procedure. The final R-value is 0.059. In the crystalline state, homotaurine molecule has the zwitterionic structure, NH_3^+–CH_2–CH_2–CH_2–SO_3^-, with *trans-zigzag* skeletal configuration, and non-hydrogen atoms except two oxygen atoms lie exactly on a mirror plane. Each molecule in the crystal is connected by three dimensional network of three NH···O hydrogen bonds.

As described in previous papers,[1-3] we have been interested in the relationship between molecular conformation and physiological action of ω-amino acids and ω-amino sulfonic acids. 3-Aminopropane sulfonic acid, homotaurine, is a structural analogue of γ-aminobutyric acid (GABA), and it has one more methylene group than taurine, 2-aminoethane sulfonic acid. As a specific inhibitor of impulse transmission in the central nervous system, the pharmacological properties and possible physiological role of GABA have been recently reviewed in detail,[4] and it has been reported that homotaurine has more potent inhibitory effect than those of taurine[4-7] and also has a hypotensive and a cardiotonic effect.[8-10] As the detailed structure of taurine was reported by Okaya,[11] we describe here the crystal and molecular structure of homotaurine, comparing its molecular conformation with that of taurine.

Experimental

The powder sample of homotaurine was kindly supplied by Prof. S. Tsunoo, School of Medicine, Showa University, Tokyo. Dissolving this sample into hot ethanol aqueous solution, it was kept cool for crystallization. We have obtained two crystallographically different crystals, α- and β-form; the former is crystallized by cooling slowly and the latter by rapid cooling. The structure analysis of β-form is now in progress and as a part of our investigation on the molecular conformation of ω-amino sulfonic acid, the report will be published in near future. Therefore, we wish to discuss here just the detailed crystal and molecular structure of the α-form.

The cell dimensions were obtained on a Rigaku Denki four circles diffractometer with Mo-$K\alpha$ radiation, and they were given in Table 1. According to the systematic absences of reflections ($h0l$; $h+l=2n+1$, $h00$; $h=2n+1$, $00l$; $l=2n+1$), the orthorhombic space groups, $P2_122_1$, $Pmnm$ and $Pmn2_1$, are all possible. In consequence of the density measurement by floatation in carbon tetrachloride and ethylene bromide mixture, the number of molecule in a unit cell is two. On the other hand, homotaurine molecule itself has no two-fold symmetry. Therefore, the space group of the crystal is determined to be $Pmn2_1$.

Table 1. Crystal data of 3-aminopropane-sulfonic acid (homotaurine)

Crystal system:	orthorhombic
Cell constants:	$a=7.059\pm0.005$ Å
	$b=5.492\pm0.006$ Å
	$c=7.428\pm0.004$ Å
Space group:	$Pmn2_1$
Density (obsd):	$D_o=1.610\pm0.002$ g/cm³
(calcd):	$D_c=1.605$ g/cm³

The prismatic crystal was cut down to be approximately $0.2\times0.2\times0.2$ mm for intensity measurement. The intensity data were collected on the Rigaku Denki computer controlled automatic four-circles diffractometer. The $\omega/2\theta$ scan technique using Zr-filtered Mo-$K\alpha$ radiation was employed. A total of 1143 independent reflections in the range of $\sin\theta/\lambda=0.95$ Å^{-1} were collected and these observed structure factors were converted into absolute values by a program for Wilson's statistics.

Structure Determination

As expected from the fact that the space group of the α-form is $Pmn2_1$ and the unit cell contains two molecules, homotaurine molecule should be located on a mirror plane.

The coordinate of sulfur atom was determined by vector relation on three Harker sections of the sharpened Patterson synthesis with coefficient of $|F_o|^2_{\text{mod.}}=$

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Table 2(a). The final fractional coordinates and their standard deviations (in Å)

	x/a	y/b	z/c	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
S	0.0	0.1178	0.2000	0.0	0.001	0.001
O (1)	0.0	−0.1260	0.1269	0.0	0.003	0.004
O (2)	0.1713	0.2549	0.1515	0.002	0.002	0.002
O (3)	−0.1713	0.2549	0.1515	0.002	0.002	0.002
N	0.0	0.5523	0.8187	0.0	0.003	0.004
C (1)	0.0	0.0908	0.4362	0.0	0.004	0.004
C (2)	0.0	0.3386	0.5291	0.0	0.004	0.004
C (3)	0.0	0.3092	0.7310	0.0	0.004	0.003
H (1)	0.142	−0.025	0.471	0.04	0.05	0.04
H (2)	−0.142	−0.025	0.471	0.04	0.05	0.04
H (3)	0.145	0.438	0.479	0.04	0.04	0.04
H (4)	−0.145	0.438	0.479	0.04	0.04	0.04
H (5)	0.147	0.221	0.784	0.04	0.04	0.04
H (6)	−0.147	0.221	0.784	0.04	0.04	0.04
H (7)	0.139	0.625	0.802	0.05	0.05	0.05
H (8)	−0.139	0.625	0.802	0.05	0.05	0.05
H (9)	0.0	0.568	0.947	0.0	0.08	0.09

Table 2(b). The final temperature factors and their standard deviations ($\times 10^4$)
The anisotropic temperature factors are in the form of $\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+\beta_{12}hk+\beta_{13}hl+\beta_{23}kl)]$

	β_{11}	σ	β_{22}	σ	β_{33}	σ	β_{12}	σ	β_{13}	σ	β_{23}	σ
S	78	1	139	2	52	1	0	0	0	0	−40	3
O (1)	235	9	166	9	114	6	0	0	0	0	−112	13
O (2)	106	3	309	8	89	3	−127	9	42	6	−33	8
O (3)	106	3	309	8	89	3	127	9	−42	6	−33	8
N	114	5	203	10	65	4	0	0	0	0	−60	12
C (1)	147	7	137	9	57	4	0	0	0	0	15	10
C (2)	128	6	159	9	56	4	0	0	0	0	−27	11
C (3)	191	9	196	11	49	5	0	0	0	0	−12	11
	β (isotropic)	σ										
H (1)	1.8	0.9										
H (2)	1.8	0.9										
H (3)	2.2	1.1										
H (4)	2.2	1.1										
H (5)	2.3	1.1										
H (6)	2.3	1.1										
H (7)	3.3	1.3										
H (8)	3.3	1.3										
H (9)	3.7	2.0										

$|F_o|^2 \exp[2\beta(\sin\theta/\lambda)^2]$. All positions of the non-hydrogen atoms were easily determined by a Fourier synthesis with phases based on the sulfur atom. After successive Fourier refinements, the discrepancy factor, $R=\Sigma||F_o|-|F_c||/\Sigma|F_o|$, decreased to 0.20.

Further refinement was carried out by the block-diagonal least-squares method. After five cycles of refinement with isotropic temperature factors ($R=$ 0.12) and further five cycles with anisotropic temperature factors for all non-hydrogen atoms ($R=0.066$), a difference Fourier synthesis was calculated to determine the locations of hydrogen atoms. Six hydrogen atoms bound to carbon atoms and two hydrogen atoms connected on the nitrogen atom were satisfactorily located with reasonable peak heights. However, peak height for the last one which was thought to be bound to the nitrogen atom was about half of others. There was also no peak to be assigned as a hydrogen atom near the sulfonic oxygen atoms on the difference map. Further five cycles least-squares refinement of positional parameters with anisotropic temperature factors for non-hydrogen atoms and isotropic for hydrogen atoms reduced the R factor to 0.059 (0.054 for $F_o \neq 0$).

The final atomic coordinates and temperature factors together with their estimated standard deviations are given in Table 2. The observed and calculated structure factors are listed in Table 3.

All the numerical calculations were carried out on a NEAC 2200—500 in the computing center of this University, a FACOM 230—60 in the data processing center at the Kyoto University and a HITAC 5020E in the computing center at University of Tokyo, using the programs written by Dr. Tamaichi Ashida and by

TABLE 3. THE OBSERVED AND THE FINAL CALCULATED STRUCTURE FACTORS

H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC
K,L=	0	0	4	40	42	5	49	49	7	22	24	K,L=	7	3	6	28	28	8	26	26	5	23	22	2	118	118	0	102	108	0	27	23
2	559	581	5*	0	0	6	18	17	8	21	22	0	61	62	7	50	51	9	22	22	6	9	13	4	103	101	1	13	19	1	36	38
4	321	318	6	23	28	7	31	31	9	17	14	1	29	28	8	4	8	K,L=	7	5	7	14	15	6	50	53	2	63	64	2	44	46
6	311	317	K,L=	10	0	8*	0	11	K,L=	8	2	2	48	45	9	31	31	0	71	73	8	9	*9	8	56	57	3	16	14	3	33	34
8	118	114	0	16	6	K,L=	9	1	0	52	53	3	21	20	10	12	7	1	28	29	K,L=	8	6	10	39	37	4	51	57	4	37	38
10	78	75	1	7	13	0	12	14	1	12	6	4	43	40	K,L=	7	4	2	71	75	0	22	23	K,L=	1	8	5	11	10	5	25	26
12	53	56	2	8	10	1	22	23	2	38	37	5	15	16	0	22	22	3	26	26	1	13	14	0	65	61	6	65	66	6	16	10
K,L=	1	0	3	20	13	2	10	6	3	12	8	6	35	39	1	54	54	4	59	61	2	15	21	1	52	51	7	16	13	7	22	21
0	155	153	K,L=	0	1	3	24	23	4	30	33	7	10	17	2	21	19	5	17	19	3	13	10	2	60	56	8	30	27	8	20	21
1	388	398	1	266	271	4	2	7	5*	0	6	8	15	19	3	43	41	6	41	42	4	15	19	3	89	91	9	5	5	K,L=	2	11
2	142	146	3	62	48	5	20	18	6	35	33	9*	0	6	4	18	12	7	20	17	5	19	9	4	50	48	K,L=	4	9	0	45	46
3	21	15	5	169	164	6	16	10	7	12	2	K,L=	8	3	5	42	41	8	29	31	6	15	16	5	38	39	0	16	14	1*	0	13
4	117	110	7	89	85	K,L=	10	1	8	21	14	0	13	20	6	8	14	K,L=	8	5	K,L=	9	6	6	43	41	1	75	77	2	43	43
5	178	176	9	29	25	0	13	9	K,L=	9	2	1	41	42	7	28	27	0	11	13	0	17	19	7	17	24	2	18	16	3	16	15
6	76	66	11	39	42	1*	0	9	0	24	23	2	23	20	8	8	9	1	26	25	1	16	17	8	29	29	3	43	44	4	36	36
7	103	99	13	21	18	2	15	9	1	10	11	3	34	33	9	17	16	2	8	11	2	15	17	9	35	33	4	18	16	5	5	13
8	42	45	K,L=	1	1	3	14	11	2	26	23	4	22	19	K,L=	8	4	3	23	22	3	9	14	10	11	17	5	60	59	6	31	31
9	26	24	0	270	269	K,L=	0	2	3	11	4	5	28	31	0	41	44	4*	0	9	K,L=	0	7	K,L=	2	8	6	7	7	7	14	6
10	30	32	1	400	418	0	458	480	4	22	21	6	15	11	1	27	27	5	22	20	1	44	32	0	77	73	7	40	41	K,L=	3	11
11	40	44	2	212	195	2	186	147	5	6	10	7	23	21	2	30	33	6	13	8	3	85	84	1	148	146	8	8	4	0	28	33
12	17	15	3	271	274	4	146	129	6	11	14	8	8	7	3	22	23	7	11	14	5	37	36	2	36	32	K,L=	5	9	1	38	35
13	18	18	4	105	89	6	179	167	K,L=	10	2	K,L=	9	3	4	32	30	K,L=	9	5	7	28	27	3	124	124	0	49	46	2	13	10
K,L=	2	0	5	169	167	8	58	51	0*	0	6	0	16	19	5	22	19	0	7	11	9	39	41	4	26	21	1	52	54	3	33	31
0	159	152	6	114	109	10	44	42	1	17	16	1	30	34	6	25	28	1	15	19	11	21	16	5	96	98	2	36	33	4	9	14
1	107	116	7	100	100	12	33	35	2*	0	8	2	20	17	7	16	13	2	4	8	K,L=	1	7	6	41	42	3	53	53	5	21	25
2	143	130	8	37	30	K,L=	1	2	3	13	16	3	31	32	K,L=	9	4	3	19	17	0	100	91	7	70	72	4	28	26	6	22	24
3	115	116	9	64	65	0	182	195	K,L=	0	3	4	11	14	0	14	18	4*	0	7	1	84	80	8	11	13	5	42	42	7	16	21
4	72	63	10	29	26	1	184	188	1	485	496	5	25	26	1*	0	2	K,L=	0	6	2	88	86	9	47	44	6	32	28	K,L=	4	11
5	99	100	11	41	37	2	166	166	3	125	115	6	10	11	2	18	17	0	130	122	3	74	71	10	9	4	7	18	26	0	19	18
6	46	43	12	28	28	3	110	103	5	217	224	K,L=	10	3	3*	0	6	2	102	111	4	74	72	K,L=	3	8	8	19	14	1	35	33
7	70	69	13	19	18	4	125	119	7	132	132	0	15	20	4	15	15	4	103	105	5	62	61	0	68	65	K,L=	6	9	2	22	19
8	38	37	K,L=	2	1	5	114	115	9	56	54	1	4	2	5	8	2	6	75	75	6	48	46	1	78	81	0	45	47	3	13	13
9	58	59	0	127	130	6	76	72	11	55	54	2	17	18	K,L=	10	4	8	52	56	7	45	47	2	59	58	1	26	22	4	19	16
10	10	12	1	53	50	7	61	63	13	25	24	K,L=	0	4	0	16	15	10	40	40	8	35	36	3	53	51	2	49	47	5	28	27
11	38	37	2	132	142	8	49	48	K,L=	1	3	0	254	248	K,L=	0	5	12	21	20	9	31	31	4	49	48	3	32	28	6	10	9
12*	0	6	3	172	168	9	14	15	0	264	259	2	146	133	1	163	154	K,L=	1	6	10	25	24	5	53	58	4	41	42	K,L=	5	11
13	16	17	4	138	132	10	33	34	1	81	85	4	120	115	3	122	121	0	48	50	11	24	19	6	42	43	5	15	13	0	39	38
K,L=	3	0	5	30	34	11	30	33	2	108	87	6	122	116	5	115	115	1	124	122	K,L=	2	7	7	42	40	6	25	28	1	27	29
0	85	89	6	95	88	12	16	18	3	80	82	8	63	60	7	69	71	2	47	46	0	126	122	8	28	30	K,L=	7	9	2	26	26
1	11	8	7	12	3	13*	0	13	4	79	70	10	42	42	9	53	55	3	163	167	1	47	48	9	14	15	0	13	14	3	27	29
2	96	96	8	64	65	K,L=	2	2	5	63	63	12	24	26	11	40	36	4	42	41	2	115	111	10	18	16	1	1	9	4	18	21
3	164	163	9	31	32	0	274	262	6	112	111	K,L=	1	4	K,L=	1	5	5	83	80	3	28	27	K,L=	4	8	2	22	23	5	21	23
4	91	90	10	45	50	1	200	188	7	42	43	0	227	226	0	158	150	6	39	40	4	89	90	0	68	72	3	10	8	K,L=	6	11
5	29	21	11	9	9	2	74	48	8	34	33	1	205	201	1	80	78	7	50	52	5	36	37	1	21	22	4	15	19	0	20	24
6	48	45	12	26	24	3	127	115	9	30	32	2	194	194	2	82	76	8	32	31	6	67	70	2	45	45	5*	0	5	1	13	8
7	42	39	13	14	0	4	49	32	10	33	30	3	191	195	3	73	73	9	49	51	7	20	15	3	23	26	K,L=	8	9	2	21	24
8	27	30	K,L=	3	1	5	92	97	11	14	19	4	148	148	4	70	66	10	25	19	8	44	47	4	37	39	0	14	18	3	12	12
9	59	59	0	175	169	6	81	77	12	28	26	5	123	121	5	64	64	11	22	22	9	2	10	5	18	19	1	20	17	K,L=	0	12
10	27	29	1	189	184	7	67	71	13*	0	10	6	107	105	6	77	73	12	11	13	10	28	27	6	49	48	K,L=	0	10	0	31	35
11	15	12	2	209	203	8	18	19	K,L=	2	3	7	70	71	7	50	50	K,L=	2	6	11	11	11	7	9	10	0	69	71	2	50	53
12	0	11	3	154	157	9	50	52	0	144	149	8	71	70	8	28	30	0	35	37	K,L=	3	7	8	27	24	2	91	95	4	41	42
K,L=	4	0	4	143	140	10	5	7	1	27	22	9	51	50	9	32	33	1	85	87	0	108	107	9	15	10	4	76	74	6	23	22
0	126	125	5	103	107	11	33	33	2	141	138	10	51	45	10	19	24	2	62	64	1	44	44	K,L=	5	8	6	40	40	K,L=	1	12
1	142	143	6	68	66	12	15	13	3	141	137	11	36	31	11	20	20	3	76	74	2	86	81	0	47	49	8	45	44	0	46	49
2	227	232	7	56	56	13	20	16	4	124	119	12	28	24	12	16	17	4	43	42	3	35	36	1	46	47	K,L=	1	10	1	26	27
3	109	112	8	80	81	K,L=	3	2	5	16	19	K,L=	2	4	K,L=	2	5	5	63	60	5	63	63	2	50	50	0	41	41	2	48	46
4	169	170	9	42	44	0	106	106	6	87	84	0	97	95	0	264	264	6	20	19	5	31	34	3	29	33	1	26	25	3	49	46
5	79	77	10	40	41	1	28	21	7	13	9	1	156	156	1	127	127	7	43	46	6	62	64	4	42	47	2	40	38	4	37	38
6	70	70	11	24	25	2	94	96	8	58	59	2	80	78	2	232	228	8	25	24	7	28	29	5	29	33	3	55	54	5	19	18
7	62	62	12	9	15	3	132	127	9	35	33	3	143	147	3	56	60	9	30	30	8	35	36	6	35	31	4	33	32	6	31	30
8	85	86	K,L=	4	1	4	81	86	10	44	43	4	50	48	4	176	174	10	6	9	9	19	18	7	24	24	5	11	13	K,L=	2	12
9	30	28	0	32	29	5	21	18	11	10	5	5	116	113	5	73	76	11	16	18	10	8	19	8	22	22	6	28	27	0	22	17
10	44	44	1	142	138	6	52	55	12	19	22	6	39	37	6	132	129	K,L=	3	6	K,L=	4	7	K,L=	6	8	7	16	17	1	34	35
11	14	14	2	35	38	7	29	29	K,L=	3	3	7	75	76	7	44	45	0	44	43	0	22	18	0	26	24	8	20	19	2	8	7
12	12	15	3	203	201	8	35	38	0	131	132	8	22	25	8	85	84	1	107	108	1	63	63	1	44	45	9	21	23	3	28	31
K,L=	5	0	4	38	41	9	45	48	1	107	102	9	56	54	9	16	16	2	42	42	2	21	10	2	38	36	K,L=	2	10	4*	0	4
0	166	164	5	88	84	10	30	30	2	121	120	10	13	8	10	49	48	3	70	65	3	44	45	3	44	44	0	39	40	5	28	25
1	57	52	6	14	9	11	14	10	3	100	99	11	32	32	11	20	18	4	40	40	4	11	10	4	29	29	1	69	69	6	14	9
2	152	152	7	68	68	12*	0	13	4	91	89	12	12	8	12	28	27	5	71	74	5	50	52	5	33	34	2*	0	1	K,L=	3	12
3	111	111	8	14	5	K,L=	4	2	5	73	72	K,L=	3	4	K,L=	3	5	6	20	24	6	5	9	6	13	12	3	56	58	0	18	19
4	115	113	9	61	64	0	71	63	6	57	57	0	97	93	0	146	147	7	50	52	7	41	40	7	17	20	4	11	7	1	47	49
5	43	38	10	13	11	1	38	38	7	38	39	1	160	159	1	111	106	8	18	17	8	8	6	K,L=	7	8	5	44	48	2	19	17
6	90	91	11	19	20	2	161	157	8	56	56	2	89	89	2	109	103	9	19	24	9	22	21	0*	0	11	6	27	24	3	26	28
7	37	38	12*	0	1	3	35	32	9	32	32	3	172	167	3	90	89	10	14	14	10	11	8	1	48	45	7	34	38	4	14	12
8	61	60	K,L=	5	1	4	116	114	10	29	27	4	79	79	4	84	81	11	25	22	K,L=	5	7	2	9	12	8*	0	2	5	39	38
9	43	43	0	44	48	5	23	21	11	16	19	5	97	98	5	78	74	K,L=	4	6	0	57	60	3	49	47	9	22	23	K,L=	4	12
10	22	27	1	92	93	6	43	41	12*	0	14	6	48	46	6	76	76	0	83	83	1	33	30	4	18	13	K,L=	3	10	0	52	57
11	13	10	2	32	23	7	15	17	K,L=	4	3	7	75	76	7	56	56	1	21	21	2	29	29	5	29	31	0	44	44	1	8	11
K,L=	6	0	3	71	70	8	63	64	0	65	68	8	27	31	8	38	43	2	65	63	3	33	33	6	17	8	1	41	42	2	42	40
0	42	47	4	16	16	9	12	9	1	114	114	9	35	37	9	35	34	3	27	23	4	24	26	K,L=	8	8	2	40	39	3*	0	8
1	60	57	5	55	58	10	32	32	2	57	63	10	22	25	10	20	22	4	53	53	5	23	26	0	1	10	3	16	13	4	33	36
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3	44	43	7	48	54	12	11	11	4	37	40	12	17	10	K,L=	4	5	6	57	58	7	22	19	2	21	15	5	26	34	0	28	27
4	11	8	8	23	22	K,L=	5	2	5	75	75	K,L=	4	4	0	26	27	7	10	9	8	5	10	3	12	7	6	30	28	1	12	16
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10*	0	5	1	48	45	5	24	24	11	21	20	5	31	30	6	10	16	1	70	70	3	28	22	7	42	41	2	37	34	K,L=	1	13
K,L=	7	0	2	63	60	6	53	55	12	13	10	6	66	66	7	47	47	2	56	54	4	57	55	9	47	44	3	39	37	0	20	23
0	41	37	3	13	11	7	19	22	K,L=	5	3	7	18	13	8	14	11	3	62	64	5	12	8	K,L=	1	9	4	31	32	1	26	25
1	51	51	4	48	48	8	37	38	0	64	59	8	56	59	9	34	35	4	47	51	6	41	39	0	71	70	5	29	30	2	29	33
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5	43	43	8	37	36	K,L=	6	2	4	68	68	K,L=	5	4	0	55	52	8	20	25	0	36	34	4	85	86	0	38	37	K,L=	2	13
6	21	21	9	10	2	0	24	25	5	49	54	0	96	96	1	48	48	9	21	24	1	20	16	5	56	57	1	31	32	0	38	37
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8	5	14	K,L=	7	1	2	32	30	7	47	48	2	92	92	3	46	48	K,L=	6	6	3	17	16	7	42	43	3	10	14	2	36	36
9	12	13	0	69	68	3	63	61	8	40	43	3	30	28	4	39	40	0	23	22	4	29	31	8	43	45	4	31	29	3	12	13
K,L=	8	0	1	44	44	4	19	22	9	25	25	4	73	76	5	37	39	1	67	68	5	12	13	9	27	27	5	23	26	4	29	31
0	43	41	2	45	43	5	48	50	10	23	21	5	36	36	6	32	31	2	23	24	6	23	20	10	24	26	6	21	20	K,L=	3	13
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2	29	26	4	40	40	7	44	45	K,L=	6	3	7	18	21	8	27	26	4	13	15	K,L=	8	7	0	68	70	0	7	6	1	23	20
3	31	30	5	23	26	8	17	14	0	48	49	8	41	41	9	23	22	5	48	50	0*	0	7	1	24	24	1	29	25	2	20	18
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7*	0	11	9	12	9	0	58	57	4	37	39	K,L=	6	4	1	51	52	9	24	23	4*	0	3	5	10	20	5	29	20	K,L=	0	14
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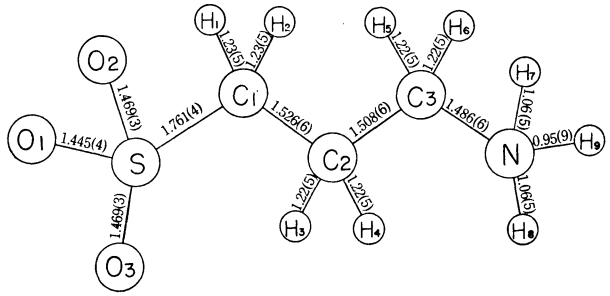
K,L=	9	0	0	30	30	2	53	53	6	34	34	1	97	98	3	62	64	0	26	20	K,L=	9	7	7	7	5	1	48	51	K,L=	1	14
0	49	49	1	70	67	3	36	35	7	11	9	2	21	19	4	50	49	1	31	29	0	14	16	8	30	30	3	75	73	0	30	32
1	7	4	2	29	28	4	39	40	8	18	25	3	87	87	5	36	34	2	17	19	1	13	14	9	16	13	5	35	36			
2	46	47	3	50	48	5	35	35	9	9	4	4	19	19	6	36	36	3	29	27	K,L=	0	8	10	10	16	7	29	27			
3	12	9	4	27	24	6	29	33	10	10	14	5	65	68	7	25	25	4	20	14	0	79	76	K,L=	3	9	K,L=	1	11			

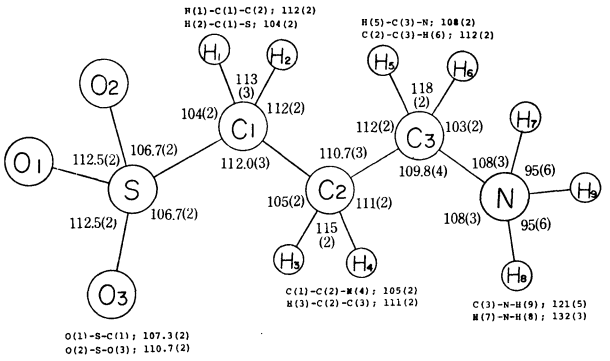
the authors.

Results and Discussion

The bond distances and angles are shown in Fig. 1 (a) and (b).



(a)



(b)

Fig. 1. (a) Bond distances and their standard deviations in parentheses (in Å).
(b) Bond angles and their standard deviations in parentheses (in degree).

In crystal of the α-form, homotaurine molecule has the zwitterionic structure NH_3^+–CH_2–CH_2–CH_2–SO_3^-, and the seven atoms, O(1), S, C(1), C(2), C(3), N and H(9), in a molecule are exactly on a mirror plane and these atoms preserve the planar *trans-zigzag* configuration, while the same zwitterionic molecule of taurine has the *gauche* configuration around the central methylene linkage. A hydrogen atom, H(9), the location of which is still obscure, should be on the mirror plane and has to be *trans* configuration to C(2) atom with respect to C(3)–N bond, participating in NH···O hydrogen bond formation with the adjacent molecule on the same mirror plane.

It is still unknown about the general feature of molecular conformation of ω-amino sulfonic acid, but such *trans-zigzag* configuration in the homotaurine molecule is also found in GABA hydrochloride[12] and γ-guanidinobutyric acid (GGBA) hydrochloride and hydrobromide,[3] which are particularly interesting substances for the investigation on the relation between their molecular conformations and their characteristic physiological actions.

The configuration of the sulfonic group is considerably interesting. O(2) and O(3) oxygen atoms in a molecule are related by the mirror plane symmetry, and have exactly equal S–O distances of 1.469 Å, whereas O(1) atom exhibits a smaller separation of 1.445 Å. Considering the fact cited above and the longer O(1)···HN hydrogen bond distance of 2.892 Å, O(1) atom might be loosely interacted with an amino group, and it may reflect the ambiguity of H(9) position. Larger C(1)–S–O bond angle was found in the shorter S–O bonds, and it was also observed in taurine.

The C(1)–S distance of 1.761 Å is very similar to that of taurine molecule.[11] Taurine is a structural analogue of homotaurine, and as shown in Table 4 one significant deviation is found in bond angle C–C–N, 109.8° in homotaurine and 112.6° in taurine, while the corresponding angle in ω-amino acids is 111.2° in GABA[13] and 108.4° in β-alanine.[14]

The intramolecular distances between sulfonic group and amino group of ω-amino sulfonic acid are shown in Table 5. Considering the fact that taurine is less active than homotaurine on depression of cortical responses.[4–7] the conformational difference between these compounds might be substantial in these physiological significances. Another interesting feature to be noted here is that NH_3^+–$\underset{|}{CH}$–CH_2–SO_3^- configuration of taurine is same as that of L-cysteic acid,[15] which is active on excitation of cortical responses,[5] and furthermore homocysteic acid which possesses NH_3^+–$\underset{|}{CH}$–CH_2–CH_2–SO_3^- group as homotaurine, has much stronger excitatory action than cysteic acid. The configuration of homocysteic acid might be same as that of homotaurine.

Table 4. A comparison of bond distances and angles between homotaurine and taurine

	Taurine[11] NH_3^+-CH_2-CH_2-SO_3^-	Homotaurine NH_3^+-CH_2-CH_2-CH_2-SO_3^-
∠OSO	110.9°, 113.0°, 113.7°	110.7°, 112.5°, 112.5°
∠CSO	105.8°, 105.8°, 106.9°	106.7°, 106.7°, 107.3°
∠SCC	112.9°	112.0°
∠CCC	—	110.7°
∠CCN	112.6°	109.8°
S-O	1.44_8, 1.46_1, 1.46_5 Å	1.44_5, 1.46_9, 1.46_9 Å
S-C	1.78_0 Å	1.76_1 Å
C-C	1.52_0 Å	1.50_8, 1.52_6 Å
C-N	1.48_4 Å	1.48_6 Å

Table 5. Intramolecular distances between sulfonic and amino group of ω-amino sulfonic acid

	N-O(1)(Å)	N-O(2)(Å)	N-O(3)(Å)
Taurine[11]	4.54	3.82	2.93
L-Cysteic acid[15]	4.41	4.11	2.84
Homotaurine	6.38	5.36	5.36

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15) H. Konishi, T. Ashida, and M. Kakudo, This Bulletin, **41**, 2305 (1968).

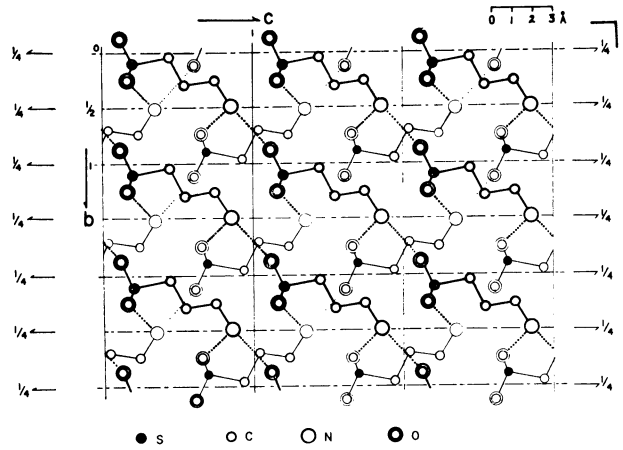

Fig. 2. (a) The crystal structure of homotaurine viewed down along the *a*-axis.

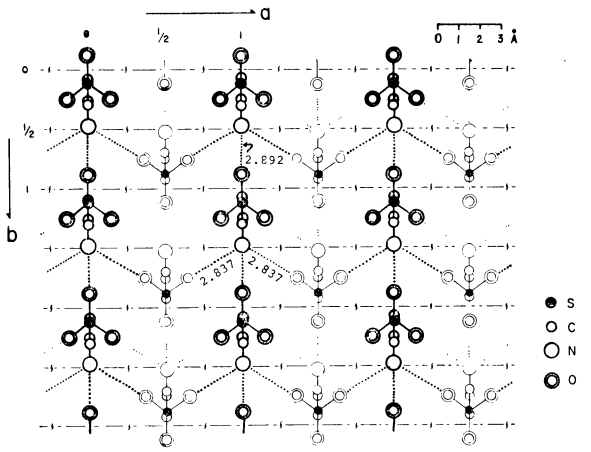

Fig. 2. (b) The crystal structure of homotaurine viewed down along the *c*-axis.

Figure 2 (a) and 2 (b) show the packing of molecules in crystal lattice projected along the *a*- and *c*-axis respectively, where the dotted lines indicate the hydrogen bonds. Homotaurine molecules are jointed to each other with three NH···O hydrogen bonds (2.837, 2.837 and 2.892 Å) to form three dimensional network structure, whereas in taurine structure, there are three NH···O intermolecular hydrogen bonds of 2.793, 2.893, and 2.939 Å, and one intramolecular hydrogen bonding of 2.926 Å. The intermolecular contacts between adjacent molecules are kept by normal van der Waals distances, of which the shortest one between N and C(2) atoms related by two-fold screw axis is 3.906 Å.

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