Crystal and Molecular Structure of ω-Amino Acids, ω-Aminosulfonic Acids and Their Derivatives. III. The Crystal and Molecular Structure of γ-Guanidino-β-hydroxypropane Sulfonic Acid

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γ-Guanidino-β-hydroxypropane sulfonic acid $C_4H_{11}O_4N_3S$ crystallizes in the monoclinic space group $P2_1/c$, with four formula units in a unit cell of dimensions, $a=7.44$, $b=9.89$, $c=11.11$ Å and $\beta=97.75°$. The crystal structure was determined by the heavy atom method and refined by block-diagonal least-squares to an R-value of 0.12 using intensity data collected photographically. The molecule takes the zwitterionic form, $(NH_2)_2{}^+CNH\text{-}CH_2CH(OH)CH_2SO_3{}^-$. The skeletal conformation of the molecule is planar *trans* zigzag. The molecules are held together in the crystal by a three-dimensional network of NH···O and OH···O hydrogen bonds.

γ-Guanidino-β-hydroxypropane sulfonic acid (GGBOPSA) is one of the derivatives of chemical transmitter in the central nervous system[1-3] such as γ-amino-butyric acid (GABA), γ-amino-β-hydroxybutyric acid (GABOB), homotaurine and taurine. This work is a part of a series of structural studies on the derivatives of the above compounds. Details of action mechanisms are not clear. However, it was reported that guanidino derivatives of ω-aminosulfonic acid such as GGBOPSA and γ-guanidinopropane sulfonic acid (GGPSA) act as a depressant for the lowering of blood pressure, whereas homotaurine and γ-amino-β-hydroxypropane sulfonic acid (GABOPSA) show an excitatory action for it.[4] It would be of great interest to elucidate the correlation between structural specificities and biological implications of these compounds.

Some structural features of GGBOPSA and its related compounds have been reported.[5] This paper deals with the precise structure analysis of GGBOPSA and comparison of the molecular structure with that of the related compounds.

Experimental

A racemic sample of GGBOPSA (supplied by Prof. S. Tsunoo, Medical School of Showa University) was recrystallized from water at room temperature as colorless, transparent prisms elongated along the a-axis. The space group and cell constants were determined from Weissenberg and precession photographs. The crystal data are presented in Table 1. Intensity data of 1452 independent reflections around a and b-axes were collected from equi-inclination Weissenberg photographs by the multiple film method with Cu$K\alpha$ radiation and estimated by visual comparison with a calibrated scale. Lorentz, polarization and spot-shape corrections were applied, but no absorption correction was made. The approximate scale factor and over-all temperature factor were calculated by Wilson's method.

TABLE 1. CRYSTAL DATA OF GGBOPSA

Molecular Formula: $C_4H_{11}O_4N_3S$	M.W.=197.21
Colorless transparent prism, Monoclinic system	
$a=7.44\pm0.02$ Å	$b=9.89\pm0.02$ Å
$c=11.11\pm0.03$ Å	$\beta=97.75\pm0.5°$
Volume of the unit cell, 810.02 Å^3	
Density (by flotation) 1.621 g cm^{-3}	
Density(calculated) 1.617 g cm^{-3}	
$Z=4$	$F(000)=416$
Absent spectra: $h0l$ when $l=2n+1$	
$0k0$ when $k=2n+1$	
Space group, $P2_1/c$	

Structure Determination and Refinement

The structure was solved by the usual heavy-atom procedure. By interpretation of high peaks on sharpened Patterson function, the coordinates of sulfur atom were easily determined. From the Fourier synthesis with only the heavy atom phase, all the non-hydrogen atoms could be found. R-index, $R=\sum||F_o|-|F_c||/\sum|F_o|$, was reduced from 0.32 to 0.18 by block-diagonal least-squares refinement with isotropic temperature factors, the unit weight being applied for the non-zero reflections. Refinement was continued with anisotropic temperature factors and R-index was reduced to 0.14. The used anisotropic temperature factors are of the form: $\exp\{-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{13}hl+B_{23}kl)\}$.

A difference Fourier synthesis calculated in this stage revealed all the hydrogen atoms which were included in the further refinement. The final R-value was 0.12. The used atomic scattering factors were taken from *International Tables for X-ray Crystallography*.[6]

All the computations were carried out on NEAC 2200-500 and 2200-700 machines at this University and on FACOM 230-60 at the University of Kyoto, using the programs of UNICS system.

Results and Discussion

The final positional and thermal parameters are listed in Tables 2-a and b, together with their estimated

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5) Y. B. Kim, A. Wakahara, T. Fujiwara, and K. Tomita, *Chem. Lett.*, **1972**, 891.
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Table 2-a. Final positional and thermal parameters with their estimated standard deviations in parentheses ($\times 10^4$)

The anisotropic temperature factors are expressed in the form of

$$\exp\{-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{13}hl+B_{23}kl)\}$$

Atom	x/a	y/b	z/c	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
S	12216(3)	950(2)	3718(2)	62(4)	18(2)	37(2)	−1(5)	44(4)	−25(3)
O(1)	12240(10)	−269(7)	2972(7)	111(14)	59(7)	82(7)	34(17)	41(16)	−111(12)
O(2)	13224(10)	2062(7)	3271(7)	86(13)	66(7)	84(7)	−38(17)	138(16)	13(12)
O(3)	12792(10)	671(7)	4996(6)	125(14)	42(6)	34(5)	20(15)	−30(13)	−1(9)
O(4)	10181(9)	3873(6)	3945(6)	86(13)	29(6)	64(6)	−30(14)	47(14)	−21(10)
C(1)	9914(12)	1461(9)	3591(8)	70(17)	30(7)	45(8)	30(19)	31(18)	−23(12)
C(2)	9597(12)	2679(8)	4408(8)	52(16)	25(7)	46(7)	−2(18)	23(17)	5(12)
C(3)	7640(13)	2772(9)	4561(9)	76(18)	28(8)	52(8)	−9(19)	60(19)	−4(12)
C(4)	6069(12)	3934(9)	6090(8)	73(17)	42(8)	28(6)	−9(20)	15(16)	−27(12)
N(1)	7362(10)	3888(7)	5370(7)	65(14)	27(6)	41(6)	−1(16)	30(14)	−13(10)
N(2)	6060(10)	5015(7)	6836(7)	67(14)	35(7)	48(6)	−11(16)	91(16)	−11(11)
N(3)	4869(11)	2987(8)	6121(7)	101(16)	40(7)	51(7)	−62(18)	71(17)	−22(12)

Table 2-b. Fractional coordinates of hydrogen atoms ($\times 10^4$)

Atom	Bound to	x	y	z	
H(1)	O(4)	9371	4211	3279	
H(2)	C(1)	8986	556	3887	
H(3)	C(1)	9596	1635	2605	
H(4)	C(2)	10178	2399	5368	
H(5)	C(3)	7328	1700	5079	Over-all isotropic
H(6)	C(3)	6938	2960	3645	temperature factor
H(7)	N(1)	8501	4679	5425	is 1.156Å²
H(8)	N(2)	5157	5227	7297	
H(9)	N(2)	6953	5635	6917	
H(10)	N(3)	4084	2982	6855	
H(11)	N(3)	4764	2383	5455	

standard deviations. The observed and calculated structure factors are listed in Table 3. Figure 1 shows bond distances and angles with the numbering of atoms. The bond lengths and angles are compared in Table 4 with those of other compounds such as L-arginine dihydrate,[7] taurine,[8,9] homotaurine,[10] GABA,[11] GABOB,[12] and γ-guanidinobutyric acid hydrochloride (GGBA·HCl).[13] Similarly, in the cases of taurine and homotaurine, the guanidyl group is protonated by one hydrogen atom of the sulfonate group, the three S–O bonds of the resultant $-SO_3^-$ group being equivalent in the state of resonance. The average O–S–O and C–S–O angles in the sulfonate group are 112.1 and 106.7°, respectively. Deviations from the tetrahedral angles are probably due to the repulsion between the adjacent oxygen atoms which lie at the short contact distances of 2.42 Å as discussed in taurine by Sutherland and Young.[8]

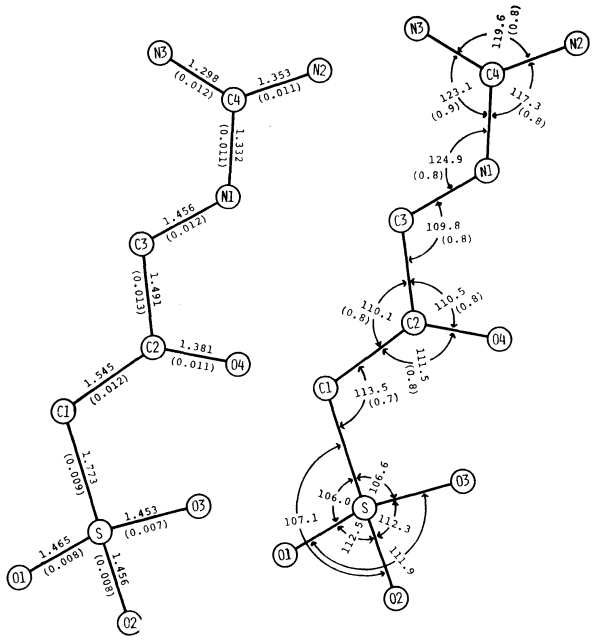

Fig. 1. Bond lengths (Å) and angles (°) of GGBOPSA. Estimated standard deviations are listed in the parentheses and those of angles around sulfur atom are 0.5°.

The guanidyl group is planar and the equation of the least-squares plane through the four atoms, N(1), C(4), N(2), and N(3), is

$$-0.51539X + 0.47909Y - 0.71053Z = -4.76419.$$

Deviations of the individual atoms from this plane are N(1): −0.0027, C(4): 0.0081, N(2): −0.0026 and N(3): −0.0028 Å. The dihedral angle between this plane and that passing through C(1)–C(2)–C(3) is 27.4°. In L-arginine dihydrate,[7] the deviations of the individual atoms from the least-squares plane of guanidyl group are N(1): −0.0005, C(4): 0.0015, N(2): −0.0005, and N(3): −0.0005 Å. Thus, the planarity of the guanidyl group in GGBOPSA is in good agreement with that of L-arginine dihydrate. All the C–N bond distances of the guanidyl group are halfway between the value of single bond (1.47 Å) and that of double bond (1.24 Å) proposed by Shomaker and

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TABLE 3. OBSERVED AND CALCULATED STRUCTURE FACTORS

K	Fo	Fc
H,L=	0	0
2	83	68
4	104	-90
6	199	-216
8	110	84
10	183	201
H,L=	0	1
1	52	-34
2	269	-302
3	141	-137
4	120	105
5	113	105
6	74	58
7	72	55
8	161	142
9	137	131
10	66	56
11	64	-67
12	37	-45
H,L=	0	2
0	173	175
1	292	330
2	176	-171
3	162	155
4	143	-134
6	221	-207
7	178	-177
9	80	-66
H,L=	0	3
1	94	74
2	224	-224
3	186	-183
4	155	-149
5	74	-51
6	76	39
7	60	-47
8	46	35
9	97	80
10	58	46
12	97	-92
H,L=	0	4
0	295	-315
1	75	-57
2	90	71
3	53	-57
4	224	240
5	94	106
6	109	94
8	46	-41
9	82	62
10	132	-140
11	37	-24
H,L=	0	5
1	88	-95
2	172	173
3	75	78
4	90	-71
5	93	-66
6	68	44
7	63	51
8	120	-123
11	67	68
H,L=	0	6
0	144	134
1	66	-51
2	105	81
3	295	-325
4	55	33
5	38	32
6	37	14
7	109	100
8	55	-40
9	36	25
11	41	-36
H,L=	0	7
1	148	-156
2	77	58
3	106	85
4	64	45
5	128	123
6	83	64
7	76	76
8	72	-60
9	54	-44
H,L=	0	8
0	141	126
1	91	69
2	86	66
3	69	-53
4	197	-218
6	125	-128
7	40	28
8	45	-33
9	23	-2
10	61	76
H,L=	0	9
1	88	-84
2	153	-149
3	84	-78
4	98	-88
5	34	29
6	79	75
7	38	37
8	48	37
H,L=	0	10
0	49	38
2	102	92
3	106	111
5	23	7
7	61	-54
8	41	-44
H,L=	0	11
1	69	57
2	64	-59
4	32	-26
5	62	-62
6	27	11
7	50	56
H,L=	0	12
0	101	-110
1	56	-60
4	50	56
6	47	60
H,L=	0	13
1	38	-39
2	49	52
3	34	27
4	29	43
H,L=	0	14
0	24	-23
1	23	-34
H,L=	1	0
1	67	-64
2	53	-29
3	174	-173
4	174	-176

K	Fo	Fc
5	42	-39
6	109	-88
7	81	67
8	96	75
9	148	174
10	83	-66
11	33	32
H,L=	1	1
1	238	-257
2	466	520
3	94	78
4	115	94
5	43	-43
6	39	32
7	90	81
8	236	-267
9	50	-30
10	37	28
11	74	-81
12	54	55
H,L=	1	2
0	567	614
1	468	523
2	168	185
3	37	-17
4	66	-50
5	136	-139
6	113	-115
7	197	-197
8	89	75
9	45	-22
10	138	159
11	77	87
12	45	51
H,L=	1	3
1	167	178
2	125	135
3	73	60
4	45	53
5	101	86
6	86	81
7	121	117
8	43	31
10	83	82
11	31	-40
12	34	-49
H,L=	1	4
0	246	-257
1	271	287
2	81	-83
3	32	37
4	82	-64
5	28	29
7	149	-150
8	62	-40
9	68	-66
11	87	100
H,L=	1	5
1	107	109
3	186	-167
4	82	-69
5	149	-150
7	127	-122
8	52	28
11	75	81
H,L=	1	6
0	140	-134
1	188	-189
2	58	44
3	141	-135
4	74	58
6	151	167
7	56	38
9	69	55
10	75	-81
11	49	-47
H,L=	1	7
1	46	51
2	107	92
3	98	95
4	133	130
5	94	-92
8	57	-46
10	38	-34
H,L=	1	8
0	44	31
1	132	-124
2	72	49
3	163	-177
4	119	-99
5	80	-81
7	86	85
9	71	83
10	35	39
H,L=	1	9
1	56	-48
3	62	52
4	109	112
7	81	82
8	37	-38
9	52	-71
H,L=	1	10
0	37	28
2	83	75
3	58	42
4	108	-112
5	50	-40
6	76	-88
H,L=	1	11
3	55	-56
H,L=	1	12
3	62	64
H,L=	1	13
1	87	82
H,L=	1	-1
1	110	120
2	299	335
3	69	-50
4	176	188
5	42	-31
6	87	-62
7	152	-146
8	112	-129
9	71	65
H,L=	1	-2
0	423	-422
1	188	-187
2	231	-258
3	251	-283
4	266	254
5	35	-24
6	139	122
10	131	-134
12	35	-41
H,L=	1	-3
1	175	174

K	Fo	Fc
2	169	-174
3	31	-35
4	167	149
5	19	19
6	92	80
7	93	-70
8	174	184
9	52	47
11	59	48
12	87	-86
H,L=	1	-4
0	178	187
1	28	3
2	112	-122
3	131	114
4	327	345
5	87	-66
6	96	78
7	95	-87
8	56	-45
9	68	-63
10	34	39
11	48	40
H,L=	1	-5
1	173	-167
2	89	-68
4	82	-85
5	168	177
6	93	73
9	83	-68
10	42	-19
11	63	-68
H,L=	1	-6
0	25	-13
1	35	12
2	104	-81
3	87	90
4	167	-158
5	99	-89
6	149	-157
8	45	-43
10	44	56
11	34	34
H,L=	1	-7
1	112	-94
2	206	220
3	47	33
4	155	139
5	124	130
6	56	-45
7	37	-30
8	88	-80
9	54	-50
H,L=	1	-8
1	53	-49
2	84	78
3	145	-157
5	87	-81
6	64	52
7	67	56
9	38	29
H,L=	1	-9
1	57	46
2	126	122
3	50	28
4	120	119
5	99	-97
6	67	-56
8	31	-34
9	37	33
H,L=	1	-10
0	141	-159
1	79	-77
2	43	-33
3	37	-23
4	97	93
6	82	87
8	33	-27
H,L=	1	-11
1	51	46
2	105	-116
4	49	-23
5	54	-55
6	61	63
H,L=	1	-12
0	54	-59
H,L=	1	-13
2	78	-83
H,L=	2	0
0	280	-279
1	93	91
2	256	-267
3	161	-181
4	42	32
5	93	95
6	165	178
7	119	122
8	64	56
10	101	-98
11	33	-23
12	40	-46
H,L=	2	1
1	107	100
2	51	43
3	130	-142
4	78	71
5	37	-29
6	105	-92
7	166	170
8	167	-169
10	37	-29
11	51	33
12	48	55
H,L=	2	2
0	165	-191
1	125	-137
2	43	-28
3	35	38
4	34	24
5	57	-46
6	30	13
7	48	36
9	146	171
11	67	-58
H,L=	2	3
1	176	-208
2	153	172
3	126	122
4	98	91
5	113	109
6	73	-63
7	102	102
8	83	-64
9	193	-185
10	50	49
11	79	-87

K	Fo	Fc
H,L=	2	4
0	144	-129
1	131	114
2	68	43
3	156	153
4	48	32
7	140	-164
9	54	-47
10	78	86
11	27	35
H,L=	2	5
1	51	33
2	49	-44
3	179	193
4	66	-62
5	89	64
6	70	-56
7	83	64
8	102	102
9	88	-90
10	45	48
11	23	-21
H,L=	2	6
0	232	-257
1	140	131
3	157	165
5	92	72
6	99	102
7	73	-61
9	94	-89
10	57	-59
H,L=	2	7
1	73	70
2	33	-30
3	76	-70
4	77	-72
5	141	-168
7	119	-137
8	36	19
9	31	30
H,L=	2	8
0	77	-75
1	77	-66
2	58	-53
5	61	-40
6	89	92
7	63	57
H,L=	2	9
1	118	129
2	37	48
4	71	72
8	39	-54
H,L=	2	10
0	66	57
1	76	-59
5	49	-36
7	54	66
8	18	39
H,L=	2	11
4	33	26
5	42	57
6	50	-57
H,L=	2	12
0	38	26
3	64	78
H,L=	2	-1
1	439	467
2	216	-200
3	162	155
4	119	-122
5	157	-137
6	131	124
7	105	-86
8	149	149
9	103	87
11	125	120
12	56	-62
H,L=	2	-2
0	82	70
1	88	90
2	88	-80
3	59	-64
4	193	200
5	126	108
6	111	100
7	79	-68
8	74	59
9	156	-178
H,L=	2	-3
1	195	-211
2	172	-187
3	22	-21
4	296	-300
5	45	-46
6	169	165
8	100	94
9	121	-124
10	44	28
11	66	-64
12	87	-85
H,L=	2	-4
0	264	-273
3	128	121
4	83	-73
5	76	67
6	162	-163
10	35	32
H,L=	2	-5
1	75	-80
2	18	12
3	117	101
4	82	62
5	203	216
6	76	-56
8	103	-89
9	112	-110
11	89	-112
H,L=	2	-6
0	138	-125
1	45	-30
3	128	-119
4	55	34
5	52	-49
6	82	59
7	83	76
8	54	32
9	81	62
11	38	-48
H,L=	2	-7
1	103	89
2	69	56
3	51	41
4	133	148
5	93	-75
6	79	-60
7	77	-59

K	Fo	Fc
8	38	-36
9	49	33
10	27	-25
H,L=	2	-8
1	77	-65
2	98	-104
3	59	-37
4	97	85
6	131	148
7	26	26
10	46	-51
H,L=	2	-9
1	124	139
2	108	-90
3	83	-81
4	134	-141
5	130	-132
6	74	51
7	85	-78
8	60	57
9	50	51
H,L=	2	-10
0	59	-51
1	53	35
2	53	-53
3	67	62
4	93	-76
5	71	55
8	37	34
H,L=	2	-11
1	60	51
2	99	-95
4	81	-81
6	74	66
H,L=	2	-12
0	86	108
1	54	48
2	71	69
4	50	-52
6	36	-44
H,L=	3	0
0	212	208
1	71	61
2	86	-72
3	173	179
4	79	-58
5	67	54
7	125	-115
8	74	57
9	130	-110
10	43	-42
11	51	-43
12	46	-20
H,L=	3	1
1	309	350
2	199	-198
3	104	95
4	47	-28
5	184	-178
6	30	-20
8	37	25
9	158	164
11	87	102
H,L=	3	2
0	114	-118
1	130	138
2	69	56
3	64	-55
4	64	48
5	70	64
6	66	54
7	135	128
8	59	43
9	59	54
10	64	-61
H,L=	3	3
1	82	-73
2	111	107
3	182	-189
4	48	-38
6	34	-28
7	74	-51
8	110	-126
H,L=	3	4
0	49	40
1	118	-118
3	130	-114
6	95	-88
7	101	83
8	92	-90
9	62	49
10	31	37
11	46	-59
H,L=	3	5
1	184	-197
3	96	78
4	66	-49
5	227	235
6	24	19
7	79	60
8	58	50
9	92	-98
H,L=	3	6
0	90	83
3	91	78
5	64	60
7	37	-28
8	76	-72
9	55	-42
10	47	50
H,L=	3	7
1	83	-85
2	166	-192
3	85	64
4	90	-85
5	101	95
8	92	104
H,L=	3	8
0	79	-75
1	59	60
3	120	128
4	66	56
5	37	36
6	73	67
9	34	-42
H,L=	3	9
1	37	31
2	38	-27
3	59	-54
5	80	-93
7	41	-29
H,L=	3	10
0	63	-66
H,L=	3	11
1	48	30
2	70	82

K	Fo	Fc
H,L=	3	12
0	95	84
3	27	-19
H,L=	3	-1
1	194	-219
2	252	-273
3	52	-37
4	173	-169
5	129	-116
6	98	86
8	174	197
10	50	34
11	29	-27
H,L=	3	-2
0	190	224
1	245	-272
2	99	101
3	177	177
4	128	-119
5	117	114
6	182	-179
9	53	-33
10	50	37
11	59	-56
H,L=	3	-3
1	139	-184
2	150	-135
3	98	-70
4	77	-60
5	254	289
6	106	-88
7	141	73
9	74	-57
10	59	-40
11	84	-99
H,L=	3	-4
1	103	-75
2	49	36
3	130	-135
4	39	14
6	82	-58
7	173	189
8	52	-37
9	58	47
10	64	63
11	45	-55
H,L=	3	-5
1	82	84
2	77	57
3	38	33
4	116	120
6	60	-47
7	40	44
8	81	-61
9	36	38
10	32	-27
11	36	32
H,L=	3	-6
0	46	45
1	51	37
2	49	-38
4	92	76
5	93	-69
6	128	108
7	52	28
9	34	10
10	58	-58
H,L=	3	-7
1	34	42
3	81	-67
4	144	-126
5	268	-264
6	52	29
7	60	-47
9	73	65
H,L=	3	-8
0	33	-37
1	100	90
2	44	46
3	193	210
4	173	-149
5	64	42
7	91	-93
8	49	37
9	69	-60
10	24	-46
H,L=	3	-9
1	35	36
2	74	-61
3	37	35
4	111	-99
7	63	60
8	73	78
H,L=	3	-10
0	111	109
1	59	55
2	132	127
3	66	50
4	101	-90
5	51	43
6	75	-67
7	60	-58
8	23	41
H,L=	3	-11
1	82	-85
2	36	33
4	49	46
5	66	61
6	58	-50
7	62	77
H,L=	3	-12
3	69	-66
H,L=	3	-13
2	46	45
H,L=	4	0
0	412	446
1	23	9
2	47	-27
3	38	32
4	118	-128
5	39	-31
6	162	-153
7	111	-88
9	48	-35
10	53	53
H,L=	4	1
1	26	-15
2	87	-74
3	98	-87
4	51	-38
5	28	-23
6	150	136
8	79	74
9	63	55
10	52	49
11	30	-30

K	Fo	Fc
H,L=	4	2
0	79	59
1	134	147
2	126	-146
3	116	108
4	53	37
7	146	-144
H,L=	4	3
1	193	185
2	41	40
3	55	-45
4	97	81
5	121	-112
6	102	-89
7	48	28
8	76	-57
9	103	109
H,L=	4	4
0	57	-46
1	26	-16
2	108	118
3	119	-113
4	84	66
6	73	59
9	65	67
10	29	-40
H,L=	4	5
1	84	-74
2	162	176
3	54	-44
4	88	74
5	34	-33
8	97	-90
H,L=	4	6
0	77	63
1	102	-97
2	59	42
3	161	-170
4	126	-138
6	104	-104
7	71	63
9	34	31
H,L=	4	7
1	111	-111
2	59	-38
3	73	72
4	50	-36
5	94	79
6	101	106
7	63	55
9	30	-39
H,L=	4	8
0	107	110
1	35	24
2	61	50
4	49	-32
7	27	28
H,L=	4	9
2	117	-126
4	54	-44
6	58	64
7	28	25
H,L=	4	10
0	65	-61
3	30	22
4	47	55
6	17	32
H,L=	4	11
1	26	27
2	25	34
3	27	-33
4	22	29
H,L=	4	12
0	24	-39
H,L=	4	-1
1	152	-183
2	40	21
3	114	-109
4	80	-59
5	184	199
6	76	51
9	60	45
10	43	-36
11	74	-94
H,L=	4	-2
0	248	266
1	81	-81
2	83	82
3	213	-251
4	47	-37
5	55	43
6	149	-137
7	178	178
8	61	48
9	69	46
10	53	58
H,L=	4	-3
1	109	96
2	143	142
3	81	63
4	146	158
5	28	26
6	110	-102
7	94	69
8	70	-66
9	72	68
10	66	-65
H,L=	4	-4
0	91	-97
1	93	-81
2	110	-95
3	81	-72
4	153	148
5	115	-119
8	34	-35
9	46	40
10	69	-69
H,L=	4	-5
1	34	-31
2	93	79
3	93	-78
4	111	101
5	224	-225
6	48	-24
7	75	-54
9	32	24
H,L=	4	-6
0	97	-82
3	259	309
4	63	40
5	118	-103
6	64	44
7	135	-151
10	83	-98
H,L=	4	-7
2	76	-58

K	Fo	Fc
3	55	40
5	133	127
6	97	-77
8	86	72
H,L=	4	-8
0	136	128
1	55	43
2	89	75
3	126	108
4	119	-98
6	35	-28
7	56	-56
9	60	-66
H,L=	4	-9
1	126	-117
2	77	61
3	50	40
4	65	54
5	113	109
6	56	-44
7	82	73
8	34	28
H,L=	4	-10
0	35	29
1	96	-82
2	42	31
3	130	-145
4	34	-30
6	42	-35
7	85	84
8	46	-68
H,L=	4	-11
1	33	-37
2	81	80
5	62	62
6	33	28
H,L=	4	-12
0	162	-150
2	41	33
3	51	-67
4	35	37
H,L=	4	-13
1	44	64
2	38	-39
H,L=	5	0
0	180	190
1	44	40
2	111	132
3	137	-154
4	102	-95
5	32	20
6	68	-42
7	56	39
8	105	115
9	92	77
10	62	64
H,L=	5	1
1	46	-65
5	66	48
6	92	94
8	73	-60
9	33	-24
10	46	48
H,L=	5	2
0	44	-28
1	121	132
2	28	12
3	60	49
4	108	-112
5	47	-36
6	86	-82
7	126	-144
10	48	45
H,L=	5	3
1	70	61
4	105	-98
5	76	-72
6	96	88
8	34	22
9	53	-44
10	49	68
H,L=	5	4
0	156	-186
1	107	124
2	72	-65
3	57	44
4	81	88
5	44	23
6	117	121
7	81	-67
8	47	-35
9	39	-36
H,L=	5	5
1	89	86
2	107	94
5	79	-73
6	71	-72
7	35	-39
8	44	-30
H,L=	5	6
0	82	-8[illegible]
1	54	-53
2	44	29
3	76	-71
5	36	-30
6	110	121
8	26	13
H,L=	5	7
2	89	96
3	44	27
4	98	106
8	36	-51
H,L=	5	8
1	71	-62
4	136	-134
5	44	-49
6	51	-56
7	27	25
H,L=	5	9
2	46	-49
H,L=	5	10
0	29	43
2	38	36
3	35	39
H,L=	5	-1
1	81	77
2	118	123
3	91	83
4	122	127
6	108	-100
7	26	-25
8	114	-127
9	42	34
10	34	-33
H,L=	5	-2
0	104	-111

K	Fo	Fc
1	80	-82
2	239	-246
3	148	-151
4	123	117
5	32	22
6	59	42
7	44	28
8	43	-29
9	68	58
10	38	-56
H,L=	5	-3
1	75	70
2	108	96
3	76	-69
4	37	26
5	88	-76
6	34	31
7	121	-146
10	32	20
H,L=	5	-4
0	150	-171
2	140	-134
3	123	122
4	287	279
5	67	-58
6	114	99
7	109	-102
8	50	-35
9	45	-44
10	72	-80
H,L=	5	-5
2	102	-104
3	31	-24
4	79	-69
5	156	180
6	72	52
7	76	-77
8	64	61
9	31	6
H,L=	5	-6
0	62	53
1	125	116
3	105	100
8	47	26
9	55	-58
H,L=	5	-7
1	89	-82
3	108	104
4	51	37
5	109	114
7	34	26
8	49	36
9	56	-56
H,L=	5	-8
0	101	85
1	117	-125
3	106	-104
4	89	-93
5	56	-44
6	85	-72
7	85	77
8	26	19
H,L=	5	-9
2	100	97
4	77	77
5	109	-110
H,L=	5	-10
0	105	-103
1	146	-149
3	49	-43
4	42	40
6	55	59
7	57	75
H,L=	5	-11
1	146	147
2	56	-54
4	29	30
5	50	-45
H,L=	5	-12
0	104	-99
3	42	54
H,L=	6	0
0	65	-65
2	143	-120
3	122	-125
5	65	61
6	86	67
7	72	94
H,L=	6	1
2	72	52
4	77	68
6	85	-71
H,L=	6	2
0	117	93
1	63	42
2	136	134
4	63	-62
H,L=	6	3
5	77	80
7	66	81
H,L=	6	4
0	109	-103
3	146	151
4	60	-67
7	80	-95
H,L=	6	5
2	100	-78
4	81	-91
5	80	-69
H,L=	6	6
0	119	-137
3	55	61
4	53	68
6	86	107
H,L=	6	8
1	59	-32
H,L=	6	-1
1	87	63
3	61	44
4	109	-95
5	93	-108
6	106	81
7	73	-82
H,L=	6	-2
0	178	-205
2	64	-61
4	126	132
5	80	82
6	106	96
H,L=	6	-3
2	169	-161
4	186	-176
6	121	132
H,L=	6	-4
1	109	108
2	93	93

K	Fo	Fc
5	91	82
6	59	-47
H,L=	6	-5
1	78	-72
2	118	-117
3	61	46
5	90	100
7	47	59
H,L=	6	-6
0	126	147
2	103	-96
4	106	-103
6	130	-130
H,L=	6	-7
2	124	115
4	72	70
7	40	-45
H,L=	6	-8
1	96	-94
6	46	59
7	41	44
H,L=	6	-9
1	154	153
3	51	-53
H,L=	6	-10
0	72	-81
3	45	45
H,L=	6	-11
2	104	-117
H,L=	7	0
0	88	-76
1	63	-55
H,L=	7	1
1	62	46
2	29	-28
5	72	-146
7	19	8
H,L=	7	2
3	100	-93
H,L=	7	3
1	85	-76
2	95	69
4	54	58
H,L=	7	4
0	81	68
2	91	79
4	50	-28
H,L=	7	5
1	54	-59
5	125	124
H,L=	7	6
3	102	99
H,L=	7	7
2	75	-85
H,L=	7	-1
1	63	64
2	144	-149
4	84	-74
H,L=	7	-2
0	139	127
2	124	111
3	59	43
H,L=	7	-3
1	99	-101
2	71	-63
H,L=	7	-4
0	124	122
4	82	-78
6	161	-152
H,L=	7	-5
1	61	-39
2	161	157
4	56	42
7	36	48
H,L=	7	-7
1	80	80
2	90	68
5	47	-66
H,L=	7	-8
0	74	-63
1	53	58
H,L=	7	-9
2	103	-101
4	36	-52
H,L=	7	-10
0	55	54
3	65	63
H,L=	8	0
0	97	96
1	79	82
H,L=	8	1
1	140	134
2	61	-49
H,L=	8	3
1	69	63
2	76	50
H,L=	8	4
1	62	-61
H,L=	8	5
1	46	-49
H,L=	8	6
2	26	31
H,L=	8	-1
1	80	-98
H,L=	8	-2
0	80	94
H,L=	8	-3
1	69	-70
2	124	130
H,L=	8	-4
0	87	-88
1	78	-90
4	81	87
H,L=	8	-5
1	75	81
2	83	58
4	77	93
H,L=	8	-6
0	79	-87
3	73	50
4	57	66
H,L=	8	-7
2	86	-85
H,L=	8	-8
0	69	72
2	59	-57
3	98	100
H,L=	9	-1
1	61	-76
H,L=	9	-2
1	62	-85
H,L=	9	-3
1	100	91

Table 4. Comparison of bond lengths (Å) and angles (°) with related compounds

Length	GGBOPSA	Homo-taurine	Taurine	L-Arginine	GGBA·HCl	GABA	GABOB
C(1)–C(2)	1.545	1.526	1.520	1.540	1.557	1.519	1.525
C(2)–C(3)	1.491	1.508	—	1.517	1.528	1.502	1.516
C(3)–N(1)	1.456	1.486	1.484	1.471	1.477	1.469	1.477
C(4)–N(1)	1.332	—	—	1.351	1.317	—	—
C(4)–N(2)	1.353	—	—	1.340	1.338	—	—
C(4)–N(3)	1.298	—	—	1.322	1.318	—	—
S–O(1)	1.465	1.445	1.461	—	—	—	—
S–O(2)	1.456	1.469	1.448	—	—	—	—
S–O(3)	1.453	1.469	1.465	—	—	—	—
S–C(1)	1.773	1.761	1.780	—	—	—	—
C(2)–O(4)	1.381	—	—	—	—	—	1.425
Angle							
O(1)–S–O(2)	112.5	112.5	113.7	—	—	—	—
O(1)–S–O(3)	111.9	112.5	110.9	—	—	—	—
O(2)–S–O(3)	112.3	110.7	113.0	—	—	—	—
C(1)–S–O(1)	106.0	107.3	105.8	—	—	—	—
C(1)–S–O(2)	107.1	106.7	106.9	—	—	—	—
C(1)–S–O(3)	106.6	106.7	105.8	—	—	—	—
S–C(1)–C(2)	113.5	112.0	112.9	—	—	—	—
C(1)–C(2)–C(3)	110.1	110.7	—	110.1	107.1	113.0	110.8
C(2)–C(3)–N(1)	109.5	109.8	112.6	111.1	107.8	111.8	109.5
C(3)–N(1)–C(4)	124.9	—	—	123.2	123.7	—	—
N(1)–C(4)–N(2)	117.3	—	—	121.0	120.9	—	—
N(1)–C(4)–N(3)	123.1	—	—	118.9	120.3	—	—
N(2)–C(4)–N(3)	119.6	—	—	120.2	118.7	—	—
C(1)–C(2)–O(4)	111.5	—	—	—	—	—	111.1
C(3)–C(2)–O(4)	110.5	—	—	—	—	—	107.0

Stevensen,[14] the average being 1.328 Å. We see from Table 4 that C–N distances of the guanidyl group differ (greater than 2σ) from those of GGBA·HCl. This difference is probably due to the difference of molecular environments, *i.e.*, GGBOPSA molecule is in free state while GGBA molecule is in hydrochloride salt state. Three C–N bonds of GGBOPSA have somewhat double bond character and calculation by Pauling's method[15] indicates that the double bond characters of C(4)–N(1), C(4)–N(2), and C(4)–N(3) bonds are 32, 25, and 43%, respectively, whereas the corresponding values for GGBA·HCl are 35, 29, and 36%.[13]

It is of interest to note that C(2)–O(4) distance of the hydroxyl group is 1.381 Å, significantly shorter than that of found in GABOB (1.425 Å) which is normal C–O single bond. Other bond distances and angles in the molecule are quite normal.

The skeletal conformation of GGBOPSA molecule (Fig. 2) is of *trans* zigzag form as found in GGBA·HCl, GABA·HCl, GABOB, and homotaurine. The torsion angles around C(1)–C(2) and C(2)–C(3), which are in the skeletal conformation of the molecules, are both almost 180° in homotaurine, GABA·HCl, and GGBA·HCl. On the other hand, the corresponding values of GGBOPSA are 161.9 and 177.8°, and those of GABOB, 173.7 and 168.8°, respectively. The effect of β-hydroxyl group in the molecule might be one of the factors influencing the restricted conformation and

Table 5. Hydrogen bond lengths (Å) and angles (°) of GGBOPSA

Bond length (Å)		Bond angle (°)	
O(4)–H(1)—O(1) (I)	2.732	C(2)–O(4)–O(1) (I)	110.4
N(1)–H(7)—O(4) (II)	2.907	C(3)–N(1)–O(4) (II)	127.0
N(2)–H(8)—O(2) (II)	2.944	C(4)–N(2)–O(2) (II)	137.0
N(2)–H(8)—O(4) (II)	3.231	C(4)–N(2)–O(4) (II)	91.7
N(2)–H(9)—O(1) (III)	3.271	C(4)–N(2)–O(1) (III)	111.9
N(3)–H(10)—O(2) (III)	2.827	C(4)–N(3)–O(2) (III)	114.4
N(3)–H(11)—O(3) (IV)	2.945	C(4)–N(3)–O(3) (IV)	150.9
(I) (2.0−*x*, 0.5+*y*, 0.5−*z*)		(II) (2.0−*x*, 1.0−*y*, 1.0−*z*)	
(III) (−1.0+*x*, 0.5−*y*, 0.5+*z*)		(IV) (−1.0+*x*, *y*, *z*)	

14) V. Shomaker and D. P. Stevensen, *J. Amer. Chem. Soc.*, **63**, 37 (1941).

15) L. Pauling, "The Nature of the Chemical Bond," 3rd. ed., Cornell University Press, Ithaca (1960), p. 232.

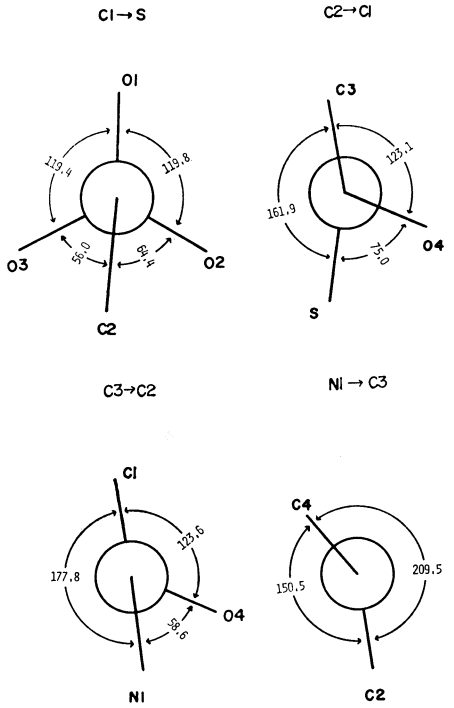

Fig. 2. Newman projection of atoms around four bonds. The arrow indicates the bond direction viewing down from front to back of paper.

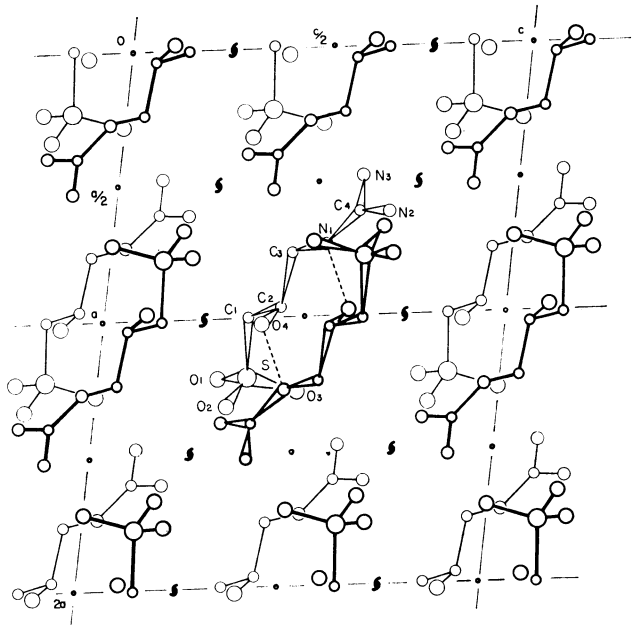

Fig. 3. The crystal structure projected along *b*-axis.

also the physiological action. Torsion angles of sulfonate group have similar values to those of homotaurine. The torsion angle around C(3)–N(1) is 150.5°, which is similar to 162.0° of L-arginine dihydrate[7] calculated.

Similarly in the case of L-arginine dihydrate, GGBOPSA molecule occurs in zwitterionic form, $(NH_2)_2^+$-$CNHCH_2CH(OH)CH_2SO_3^-$.

Distances and angles of hydrogen bonds are listed in Table 5. As shown in Fig. 3, *d*- and *l*-forms of GGBOPSA molecules were dimerized through the N(1)–H···O(4) hydrogen bonds (2.907 Å) related by a center of symmetry. This cyclic *d*–*l*, dimerization can be also seen in GABOB,[12] which were dimerized through OH···O hydrogen bond between β-OH group and oxygen atom of carboxyl group related by a center of symmetry. In these cases, however, the oxygen atom, O(4), of β-hydroxyl group of GGBOPSA molecule takes part in the intermolecular hydrogen bond system as an acceptor, while β-OH of GABOB is used to form intra- and intermolecular bifurcated hydrogen

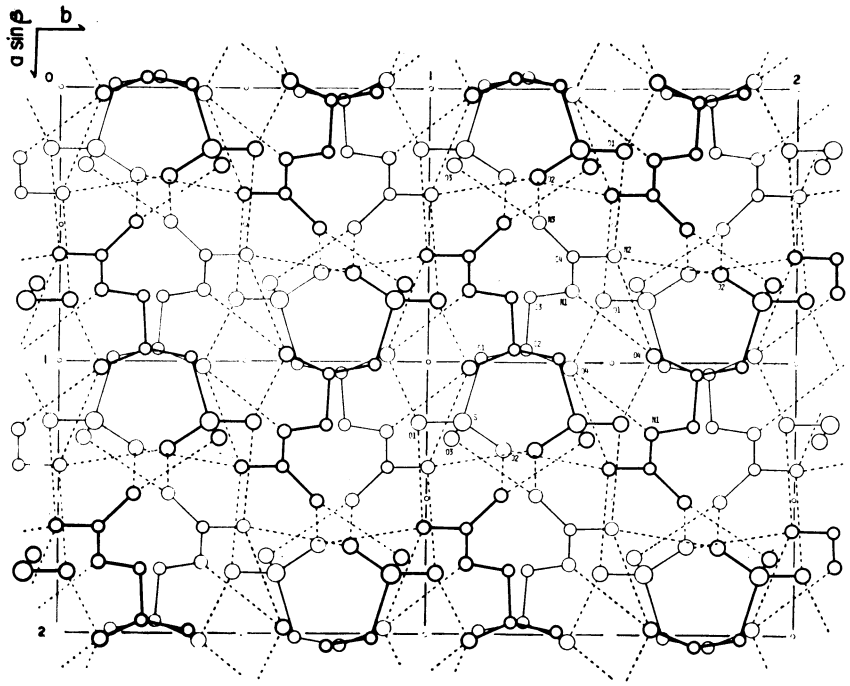

Fig. 4. The crystal structure projected along *c*-axis. The broken lines indicate the hydrogen bonds.

bond as a donor.

The crystal structure projected downward to *c*-axis is shown in Fig. 4. Among the hydrogen atoms in the molecule, all the feasible ones are utilized to form hydrogen bonds and the molecules are held together by three-dimensional network of NH···O and OH···O hydrogen bonds. The guanidyl group is connected with three neighboring molecules by six hydrogen bonds, the sulfonate group acting as an acceptor of five hydrogen bonds, and oxygen atom of hydroxyl group as both acceptor and donor. The distances of N(2) to O(2) and to O(4) by a translational operation (2.0-*x*, 1.0-*y*, 1.0-*z*) are 2.994 and 3.231 Å, respectively, H(8) atom being located on a line bisecting these two directions. Thus, the H(8) atom seems to contribute to form a bifurcated hydrogen bond. On the other hand, homotaurine molecules are jointed with each other with three NH···O hydrogen bonds to form a three-dimensional network, while in taurine, there are three NH···O intermolecular hydrogen bonds and one intramolecular hydrogen bonding. The intermolecular contacts between adjacent molecules are kept by normal van der Waals distances.

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