Crystal and Molecular Structure of ω-Amino Acids, ω-Aminosulfonic Acids and Their Derivatives. V. Crystal and Molecular Structure of γ-Guanidino Propane Sulfonic Acid

Yang Bae KIM,* Akio WAKAHARA, Takaji FUJIWARA, and Ken-ichi TOMITA

Faculty of Pharmaceutical Sciences, Osaka University, Toneyama, Toyonaka, Osaka 560

(Received March 8, 1973)

The crystal structure of γ-guanidino propane sulfonic acid was determined by the symbolic addition method with X-ray intensity data on a diffractometer and refined by the least-squares method to an *R*-value 0.069 for 1963 reflections. The crystals were monoclinic, space group $P2_1/c$, $Z=8$, with $a=10.080$, $b=8.013$, $c=19.716$ Å and $\beta=98.17°$. Two independent molecules in the asymmetric unit both have a zwitterionic form, $(NH_2)_2^+$-$CNHCH_2CH_2CH_2SO_3^-$. There are two forms, *trans* zigzag and *cis* ones, which are linked by N(1)H···O hydrogen bonds. The molecules are held together in the crystal by a three-dimensional network of NH···O hydrogen bonds.

γ-Guanidino propane sulfonic acid (GGPSA) is a guanidyl derivative of 3-amino propane sulfonic acid, homotaurine, which has strong activity towards the behavior of neurones when applied extracellularly.[1] Short-chain ω-guanidino acids and homotaurine also depress cortical responses.[2-3] Tsunoo *et al.* reported that homotaurine and γ-amino-β-hydroxy propane sulfonic acid (GABOPSA) act to lower blood pressure, and GGPSA and γ-guanidino-β-hydroxy propane sulfonic acid (GGBOPSA) acts to depress the lowering of blood pressure.[4]

It is of interest to investigate systematically the molecular structure of such compounds and elucidate the relationship between the molecular conformations and their physiological actions.

We previously reported the crystal data of GGBOPSA, GGPSA and γ-guanidino-β-hydroxybutyric acid (GGBOBA),[5] and the molecular and crystal structure of GGBOPSA.[6]

In this paper, we describe a detailed molecular and crystal structure of γ-guanidino propane sulfonic acid (GGPSA) and compare it with that of ω-amino sulfonic acids and amino acid containing guanidyl group, L-arginine.[7]

Experimental

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

Crystallographic Measurement. The space group was determined from Weissenberg and precession photographs, and lattice costants were obtained from precise measurement of the 2θ angles for 9 reflections on a diffractometer with Cu*K*α radiation. Density was measured by the flotation method in a mixture of ethylene dibromide and acetonitrile.

Table 1. CRYSTAL DATA

Molecular formula; $C_4H_{11}N_3O_3S$. M.W. 181.2,	
Colorless transparent prism, Monoclinic system	
$a = 10.080(3)$ Å	$b = 8.013(8)$ Å
$c = 19.716(1)$ Å	$\beta = 98.17(3)°$
Volume of unit cell,	1576.3 Å^3
Density (by flotation)	1.518 g/cm^3
Density (calculated)	1.522 g/cm^3
$Z = 8$	F(000) = 768
Absent spectra; *h0l* when $l = 2n + 1$	
0k0 when $k = 2n + 1$	
Space group; $P2_1/c$ with two independent molecules in an asymmetric unit.	

The crystal data are listed in Table 1.

Three-dimensional intensity data were collected on a computer controlled four-circle diffractometer (Rigaku Denki Co. Ltd.) with Ni-filtered Cu*K*α radiation using a crystal mounted about the *b*-axis. A total of 1963 independent reflections limited within $\sin\theta/\lambda<0.53$ Å^{-1} was scanned by a ω-2θ technique at a scan speed of 4° per minute. During the course of data collection, the intensities for three standard reflections 020, 006, and 500 were measured every 50 reflections in order to check the stability of the electronics or the damage on crystal lattice. All the reflections were recorded and corrected for usual Lorentz and polarization effects, no absorption correction being made.

Structure Determination and Refinement. An approximate scale and the over-all temperature factor were calculated by Wilson's method. The structure determination was tried at first by a heavy atom procedure, but there was some trouble in interpreting the Patterson function owing to too many large peaks. Failing in this, we tried to determine the structure by means of the symbolic addition method proposed by Karle and Karle.

Normalized structure factor, $|E|$, and $\sum_2$ lists ($|E|\geqq1.5$, probability greater than 97%) were calculated by the program "SIGMA" written by T. Ashida. Three-dimensional *E*-maps of 8 possible cases were calculated from the sign relations between four symbols A to D, for 145 reflections. One of them gave the positions of two sulfur atoms reasonably coincident with the corresponding coordinates in the Patterson functicn. The positions of all the non-hydrogen atoms were found by the following Fourier synthesis with phases of only two heavy atoms. An *R*-index, $\sum||F_o|-|F_c||/\sum|F_o|$, was reduced from 0.32 to 0.27 by successive syntheses with

* Present address: College of Pharmacy, Seoul National University, Seoul, Korea.

1) D. R. Curtis and J. C. Watkins, *J. Neurochem.*, **6**, 117 (1960).
2) D. P. Purpura, M. Girado, and H. Grundfest, *Science*, **127**, 1179 (1958).
3) D. R. Curtis and J. C. Watkins, *Nature*, **191**, 1010 (1961).
4) S. Tsunoo, K. Horisaka, H. Tanaka, T. Chida, S. Nakajima, and Z. Fukai, *J. Showa Med. Assoc.*, **30**, 521 (1970).
5) Y. B. Kim, A. Wakahara, T. Fujiwara, and K. Tomita, *Chem. Lett.*, **1972**, 891.
6) Y. B. Kim, A. Wakahara, T. Fujiwara, and K. Tomita, This Bulletin, **46**, 2194 (1973).
7) I. L. Karle and J. Karle, *Acta Crystallogr.*, **17**, 835 (1964).

a constant over-all temperature factor. Refinement was carried out for all reflections by the block-diagonal least-squares procedure with unit weight. The R-index was reduced to 0.14 with isotropic temperature factors for all non-hydrogen atoms and decreased further with anisotropic temperature factors to 0.11. In this state, a calculated difference Fourier synthesis (Fig. 1) revealed the locations of all the twenty-two hydrogen atoms. They were included in the final least-squares cycles with anisotropic temperature factors for non-hydrogen atoms and isotropic one for hydrogen atoms. The final R-value was 0.069. The observed and calculated structure factors for each reflection are listed in Table 2.

Calculations were carried out on an NEAC 2200—700 computer, this University, and a FACOM 230—60 computer, University of Kyoto. The scattering factors were taken from

TABLE 2. OBSERVED AND CALCULATED STRUCTURE FACTORS[a)]

K	Fo	Fc
H,L=	0	0
2	252	-277
4	18	20
6	92	-94
8	66	68
H,L=	0	1
1	68	67
2	293	355
3	151	-151
4	39	43
5	19	19
6	52	-48
7	4	6
8	9	-12
H,L=	0	2
1	59	-56
2	252	-279
3	14	-11
4	162	160
5	41	-38
6	40	-38
7	19	22
8	7	-9
H,L=	0	3
1	60	56
2	107	-107
3	20	-19
4	39	37
5	22	-21
6	69	69
7	27	27
8	19	24
H,L=	0	4
0	221	243
1	109	-112
2	198	-205
3	96	95
4	95	90
5	77	-79
6	27	-22
7	12	12
8	48	54
H,L=	0	5
1	85	-84
2	46	-39
3	66	63
4	15	-12
5	68	71
6	44	-47
7	58	-57
8	16	17
H,L=	0	6
0	102	96
1	219	-237
2	186	-188
3	58	55
4	113	107
5	24	-25
6	67	-68
7	59	59
8	2	-3
H,L=	0	7
1	71	69
2	40	36
3	8	-8
4	16	17
5	23	-22
6	19	-17
7	8	3
H,L=	0	8
0	65	-64
1	29	11
2	58	59
3	157	150
4	65	61
5	84	-82
6	7	8
7	5	-5
H,L=	0	9
1	105	-101
2	19	-14
3	61	58
4	26	25
5	28	28
6	9	-11
7	40	-41
H,L=	0	10
0	22	-8
1	100	-98
2	78	-69
3	46	42
4	28	-26
5	11	10
6	12	12
7	31	32
H,L=	0	11
1	63	58
2	4	0
3	49	-46
4	17	-12
5	4	-2
6	29	-28
7	27	27
H,L=	0	12
0	9	-6
1	15	-13
2	84	82
3	57	52
4	27	-27
5	64	-59
6	7	8
H,L=	0	13
1	25	-21
2	26	-24
3	8	4
4	11	9
5	8	7
6	4	4
H,L=	0	14
0	41	-36
1	4	3
2	43	42
3	44	-43
4	61	-61
5	31	33
6	29	29
H,L=	0	15
1	16	15
3	12	-13
4	3	-1
5	9	11
H,L=	0	16
0	54	-52
1	5	2
2	61	62
3	31	-33
4	4	-1
5	19	21
H,L=	0	17
1	8	-8
2	51	-49
3	24	-25
4	39	39
H,L=	0	18
0	18	-18
1	23	23
2	11	10
3	27	-28
4	65	-67
H,L=	0	19
1	19	19
2	26	28
3	4	-5
H,L=	0	20
0	23	-23
1	47	50
2	9	-11
H,L=	1	0
0	42	-44
1	22	20
2	42	-44
3	21	-27
4	62	-65
5	103	103
6	48	50
7	27	-24
8	10	-9
H,L=	1	1
1	109	107
2	27	-28
3	11	12
4	3	-5
5	19	-18
6	62	-63
7	51	53
8	2	-5
H,L=	1	2
0	34	-25
1	170	176
2	124	124
3	84	-80
4	62	-57
5	50	52
6	20	20
7	55	-57
8	12	-15
H,L=	1	3
1	55	-51
2	46	-48
3	54	-53
4	22	17
5	72	-76
6	6	-9
7	13	14
H,L=	1	4
0	203	218
1	60	57
2	45	28
3	6	-8
4	38	-37
5	52	50
6	16	-12
7	33	-33
8	27	29
H,L=	1	5
1	17	18
2	47	50
3	7	7
4	7	-8
5	9	9
6	24	-23
7	12	16
8	33	31
H,L=	1	6
0	96	-96
1	73	74
2	78	76
3	110	-103
4	16	13
5	19	17
6	53	-57
7	28	-29
8	13	-12
H,L=	1	7
1	63	-62
2	13	12
3	30	27
4	45	43
5	35	-35
6	67	68
7	8	5
H,L=	1	8
0	107	-104
1	27	30
2	23	-15
3	61	-62
4	3	-1
5	23	20
6	20	21
7	16	-16
H,L=	1	9
1	20	19
2	4	-2
3	50	49
4	36	-35
5	30	30
6	54	-50
7	14	-13
H,L=	1	10
0	18	-15
1	22	-27
2	37	-34
3	19	20
4	80	73
5	10	-12
6	39	-37
7	8	10
H,L=	1	11
1	13	-11
2	11	10
3	47	-49
4	11	-12
5	3	1
6	18	18
7	12	-13
H,L=	1	12
0	4	5
1	89	87
2	44	39
3	36	33
4	7	-7
5	37	-35
6	9	-8
H,L=	1	13
1	23	-20
2	59	58
3	64	62
4	6	4
5	19	20
6	15	-13
H,L=	1	14
0	55	-55
1	88	-86
2	26	-24
3	24	23
4	7	4
5	4	5
6	10	-9
H,L=	1	15
1	38	38
2	21	-22
3	58	-57
4	12	12
5	14	-15
H,L=	1	16
0	20	-19
1	30	-31
2	22	20
3	79	81
4	18	17
5	39	-40
H,L=	1	17
1	29	-29
2	77	-79
3	29	27
4	4	-5
H,L=	1	18
0	38	45
1	81	-92
2	45	43
3	16	-17
H,L=	1	19
1	25	23
2	38	35
H,L=	1	20
0	78	-77
1	37	-41
H,L=	2	0
0	42	-45
1	360	-448
2	115	120
3	5	-4
4	94	-94
5	16	-14
6	21	-22
7	53	58
8	29	-31
H,L=	2	1
1	189	197
2	112	108
3	76	-77
4	111	112
5	37	-34
6	5	7
7	12	11
H,L=	2	2
0	136	-141
1	101	101
2	74	-76
3	161	169
4	59	59
5	102	-102
6	66	70
7	13	-15
8	6	-4
H,L=	2	3
1	81	-90
2	8	6
3	69	77
4	62	-72
5	63	73
6	3	-1
7	31	-41
8	3	-3
H,L=	2	4
0	91	-197
1	79	-135
2	30	39
3	49	63
4	73	-119
5	4	2
6	40	40
7	51	53
8	13	-11
H,L=	2	5
1	73	69
2	37	38
3	66	-63
4	42	-43
5	26	-26
6	39	-40
7	36	35
8	6	5
H,L=	2	6
0	8	-5
1	5	-3
2	172	171
3	63	59
4	58	-52
5	44	-41
6	42	41
7	8	-10
H,L=	2	7
1	28	28
2	32	-32
3	64	-61
4	2	-3
5	2	0
6	21	21
7	16	-15
H,L=	2	8
0	102	98
1	35	-32
2	13	9
3	24	23
4	117	-114
5	12	14
6	24	24
7	13	-13
H,L=	2	9
1	45	39
2	80	78
3	40	-37
4	20	18
5	19	22
6	19	-18
7	5	6
H,L=	2	10
0	120	-121
1	12	-11
2	54	54
3	22	-20
4	12	16
5	14	13
6	46	45
7	15	-16
H,L=	2	11
1	18	-18
2	88	-84
3	25	-24
4	21	-23
5	18	18
6	47	49
H,L=	2	12
0	38	35
1	44	41
2	15	11
3	56	-56
4	78	-72
5	13	14
6	1	-4
H,L=	2	13
1	5	-4
2	85	83
3	39	37
4	14	13
5	8	8
6	45	-45
H,L=	2	14
0	87	-83
1	13	-12
2	10	5
3	10	-8
4	91	91
5	20	20
H,L=	2	15
1	11	-10
2	49	-48
3	9	-4
4	13	13
5	5	-2
H,L=	2	16
0	12	17
1	56	57
2	23	-26
3	10	-10
H,L=	2	17
1	21	-21
2	15	17
3	43	43
4	6	4
H,L=	2	18
0	15	14
1	23	-22
2	26	-25
3	35	-36
H,L=	2	19
1	23	24
2	24	-25
H,L=	3	0
0	61	66
1	31	-26
2	66	-69
3	18	-21
4	95	93
5	1	1
6	53	-51
7	1	0
8	11	10
H,L=	3	1
1	85	-82
2	68	-70
3	35	-36
4	24	-25
5	14	-14
6	69	72
7	4	-3
8	18	-17
H,L=	3	2
0	218	230
1	113	-112
2	78	-78
3	12	-9
4	39	39
5	25	-23
6	35	-35
7	35	36
8	37	39
H,L=	3	3
1	23	19
2	50	49
3	54	49
4	43	-44
5	14	-13
6	20	20
7	12	12
H,L=	3	4
0	130	-143
1	134	-140
2	32	27
3	55	52
4	43	44
5	37	-39
6	18	-20
7	14	16
H,L=	3	5
1	32	-41
2	39	-47
3	9	-10
4	28	27
5	20	-18
6	38	40
7	21	22
H,L=	3	6
0	107	105
1	111	-105
2	81	-77
3	106	105
4	5	3
5	80	-80
6	16	-16
7	20	19
H,L=	3	7
1	35	32
2	65	66
3	57	55
4	4	2
5	35	35
6	23	-23
7	31	-30
H,L=	3	8
0	108	-105
1	135	-132
2	11	-8
3	70	66
4	5	-3
5	2	0
6	33	35
7	38	39
H,L=	3	9
1	38	32
2	43	-41
3	70	-64
4	33	-35
5	71	-69
6	1	0
7	60	60
H,L=	3	10
0	31	26
1	3	-1
2	96	96
3	110	107
4	71	-71
5	73	-70
6	17	16
H,L=	3	11
1	24	-21
2	8	5
3	40	41
4	7	6
5	13	9
6	6	-8
H,L=	3	12
0	3	2
1	67	-69
2	27	26
3	5	4
4	57	-54
5	14	-13
6	4	5
H,L=	3	13
1	14	13
2	63	60
3	11	-11
4	6	-5
5	37	-36
H,L=	3	14
0	162	-164
1	34	34
2	90	88
3	15	14
4	7	-4
5	22	-20
H,L=	3	15
1	37	-34
2	50	-48
3	62	60
4	14	-16
H,L=	3	16
0	41	-40
1	23	20
2	51	50
3	27	-25
4	54	-54
H,L=	3	17
1	41	-40
2	39	39
3	26	25
H,L=	3	18
0	70	-72
1	10	9
2	50	49
H,L=	4	0
0	113	114
1	71	75
2	7	3
3	38	-38
4	33	33
5	4	-3
6	9	-8
7	31	-32
H,L=	4	1
1	49	58
2	5	-5
3	18	22
4	41	41
5	37	-34
6	5	8
7	8	-8
H,L=	4	2
0	16	16
1	16	11
2	76	-71
3	63	56
4	72	-68
5	57	59
6	14	11
7	26	-24
H,L=	4	3
1	26	-22
2	23	25
3	4	3
4	17	-14
5	6	4
6	40	-37
7	21	20
H,L=	4	4
0	14	5
1	19	22
2	9	2
3	86	-84
4	112	112
5	60	61
6	30	-31
7	20	-22
H,L=	4	5
1	65	-62
2	144	-140
3	2	-1
4	10	2
5	13	-11
6	55	53
7	4	1
H,L=	4	6
0	121	127
1	39	-31
2	51	-49
3	78	-74
4	12	-8
5	38	36
6	48	-51
7	22	-21
H,L=	4	7
1	8	6
2	22	26
3	26	27
4	27	33
5	4	-4
7	6	-8
H,L=	4	8
0	21	-15
1	13	13
2	13	-13
3	63	-60
4	72	71
5	37	36
6	22	-20
H,L=	4	9
1	17	19
2	16	-14
3	6	-11
4	17	14
5	16	-15
6	13	13
H,L=	4	10
0	54	51
1	75	73
2	105	-103
3	24	25
4	34	32
5	2	-6
6	19	-19
H,L=	4	11
1	26	-26
2	14	12
3	13	12
4	22	-17
5	45	47
6	15	-14
H,L=	4	12
0	98	98
1	5	-2
2	38	-39
3	49	-48
4	29	28
5	5	1
H,L=	4	13
1	59	58
2	53	51
3	52	-51
4	25	-23
5	45	-46
H,L=	4	14
0	4	2
1	84	86
2	23	-23
3	48	51
4	24	25
H,L=	4	15
1	31	-31
2	9	-10
3	37	37
4	5	-4
H,L=	4	16
0	67	66
1	50	-54
2	30	-28
3	2	1
H,L=	4	17
1	12	13
2	7	9
H,L=	4	18
0	13	-13
H,L=	5	0
0	74	-69
1	29	-27
2	54	51
3	76	71
4	41	-42
5	83	-82
6	29	30
7	27	28
H,L=	5	1
1	48	-43
2	55	52
3	100	94
4	6	-8
5	18	13
6	39	-41
7	14	-15
H,L=	5	2
0	155	-161
1	45	-43
2	79	75
3	10	-7
4	7	-6
5	15	-15
6	25	22
7	18	20
H,L=	5	3
1	33	34
2	25	22
3	35	-37
4	19	-18
5	36	-35
6	19	19
7	3	-3
H,L=	5	4
0	89	-104
1	108	118
2	84	82
3	43	48
4	47	-50
5	28	-28
6	17	19
7	2	-5
H,L=	5	5
1	48	-39
2	4	1
3	98	92
4	23	-20
5	21	19
6	16	18
7	6	-4
H,L=	5	6
0	147	-145
1	51	-50
2	130	128
3	50	-47
4	121	-120
5	44	40
6	39	37
H,L=	5	7
1	34	30
2	15	17
3	48	-42
5	47	-46
6	19	-18
H,L=	5	8
0	102	-105
1	90	82
2	83	75
3	29	-23
5	42	42
6	35	35
H,L=	5	9
1	20	-19
2	89	-89
3	4	-5
4	24	-25
5	40	39
6	63	62
H,L=	5	10
0	40	39
1	43	41
2	59	58
3	94	-92
4	110	-111
5	34	34
H,L=	5	11
1	6	5
2	80	83
3	28	-28
5	2	-1
H,L=	5	12
0	92	-103
1	69	72
2	40	42
3	66	-61
4	6	6
5	22	19
H,L=	5	13
1	34	34
2	20	-19
3	11	-11
4	5	-4
H,L=	5	14
0	23	21
1	96	93
2	20	-21
3	29	-27
4	33	-32
H,L=	5	15
1	21	-20
2	35	35
3	4	-2
H,L=	5	16
0	7	0
1	26	25
2	4	4
H,L=	6	0
0	106	98
1	26	-20
2	59	-55
3	32	-31
4	31	-26
5	6	-4
6	43	-43
H,L=	6	1
1	37	32
2	82	81
3	2	3
4	25	-20
6	3	-2
H,L=	6	2
0	13	10
1	19	14
2	39	-40
3	21	19
4	98	106
5	6	-6
6	26	-27
H,L=	6	3
1	27	-27
2	8	2
3	24	-29
4	31	-36
5	27	28
6	19	20
H,L=	6	4
0	1	1
1	14	-11
2	34	-32
3	63	65
4	34	32
5	86	-82
6	27	-30
H,L=	6	5
1	53	-53
2	43	39
3	43	41
4	15	-11
5	44	42
6	5	0
H,L=	6	6
0	7	-2
1	110	-105
2	1	-2
3	3	2
4	42	42
5	27	-26
6	19	-19
H,L=	6	7
1	73	70
3	54	-50
4	14	15
6	6	5
H,L=	6	8
0	33	31
1	22	-26
2	58	-56
3	99	100
4	4	-1
5	41	-39
H,L=	6	9
1	9	6
2	9	-12
3	5	-4
4	8	-2
5	36	37
H,L=	6	10
0	7	9
1	80	-83
2	27	26
3	46	43
4	25	-28
5	2	-2
H,L=	6	11
1	5	-2
2	22	-19
3	41	-42
4	6	6
H,L=	6	12
0	6	-3
1	66	-65
2	6	4
3	19	23
4	11	-9
H,L=	6	13
1	27	25
2	32	-33
3	21	-20
H,L=	6	14
0	22	24
1	22	-21
2	21	19
H,L=	6	15
1	17	-16
H,L=	7	0
0	23	21
1	49	42
2	18	16
3	77	-76
4	75	-71
5	46	42
6	50	48
H,L=	7	1
1	46	43
2	74	70
3	73	-69
4	52	-49
5	34	-32
H,L=	7	2
0	40	-41
1	70	66
2	28	30
3	5	9
4	3	-5
5	15	-16
6	10	9
H,L=	7	3
1	11	7
2	39	-36
3	18	22
4	13	-15
5	24	23
6	17	18
H,L=	7	4
0	42	47
1	23	25
2	6	2
3	28	-33
4	34	-34
5	34	36
H,L=	7	5
1	24	-25
2	63	59
3	15	-12
4	20	-15
5	19	19
H,L=	7	6
0	43	-41
1	38	38
2	10	-9
3	71	-65
4	71	64
5	36	33
H,L=	7	7
1	11	10
2	46	-41
3	11	6
4	3	-1
5	10	-9
H,L=	7	8
0	44	36
1	25	22
2	24	-18
3	12	13
4	7	5
H,L=	7	9
1	47	-45
2	21	16
3	19	18
4	19	19
H,L=	7	10
0	21	22
1	17	-18
2	36	-33
3	55	-54
4	44	41
H,L=	7	11
1	53	53
2	8	-11
3	19	-22
H,L=	7	12
0	40	39
1	37	36
2	52	-49
H,L=	7	13
1	24	-22
H,L=	8	0
0	23	33
1	89	-114
2	31	-36
3	23	26
4	25	27
5	32	-36
H,L=	8	1
1	49	64
2	2	-4
3	46	-51
4	15	12
5	14	-16
H,L=	8	2
0	2	-2
1	32	-30
2	6	-4
3	129	121
4	32	-29
5	58	-52
H,L=	8	3
1	25	-24
3	3	-1
4	16	15
5	32	28
H,L=	8	4
0	12	15
1	50	-48
2	23	21
3	10	9
4	28	-30
5	17	-20
H,L=	8	5
1	19	15
2	13	17
3	19	-15
H,L=	8	6
0	86	-84
1	14	-15
2	37	35
3	19	21
4	18	-13
H,L=	8	7
1	3	0
2	56	-53
3	33	33
4	23	21
H,L=	8	8
0	8	-11
1	18	-20
2	46	46
H,L=	8	9
1	8	-10
2	10	11
3	13	-11
H,L=	8	10
0	33	-47
1	39	41
2	14	16
H,L=	8	11
1	22	-22
H,L=	9	0
0	11	18
1	11	-20
2	38	-35
3	28	-26
4	55	51
H,L=	9	1
1	24	23
2	49	-45
3	17	-17
4	5	2
H,L=	9	2
0	53	52
1	39	41
2	18	-17
3	13	-12
4	16	-16
H,L=	9	3
1	23	-19
2	49	48
3	22	19
H,L=	9	4
0	23	-20
1	12	-11
2	7	-7
3	5	3
H,L=	9	5
1	16	16
2	6	-9
3	11	-11
H,L=	9	6
1	9	10
2	12	-12
H,L=	9	7
1	10	-12
2	8	9
H,L=	9	8
0	3	2
1	12	-11
H,L=	10	0
0	77	-78
1	9	8
2	39	37
H,L=	10	1
1	2	3
2	35	-34
H,L=	10	2
1	15	20
2	45	47
H,L=	10	3
1	9	-12
H,L=	10	4
0	31	-43
1	3	7
H,L=	1	-1
1	61	-56
2	59	-60
3	23	24
4	61	65
5	21	22
6	23	-25
7	23	-23
8	3	1
H,L=	1	-2
0	55	-49
1	128	123
2	64	-61
3	63	-57
4	22	-23
5	48	48
6	51	54
7	77	-79
8	23	-25
H,L=	1	-3
1	136	131
2	140	-137
3	20	13
4	82	80
5	9	-5
6	24	23
7	23	23
8	3	-3
H,L=	1	-4
0	192	-198
1	122	-120
2	82	75
3	143	-135
4	6	-3
5	93	92
6	55	52
7	8	-3
8	52	-55
H,L=	1	-5
1	151	-146
2	27	-26
3	65	60
4	80	76
6	27	-24
7	43	-45
8	7	6
H,L=	1	-6
0	50	49
1	41	44
2	110	108
3	60	-57
4	78	-70
5	46	-46
6	11	10
7	7	3
8	21	-24
H,L=	1	-7
1	34	34
2	98	-92
3	12	-10
4	61	-60
6	35	36
7	43	45
H,L=	1	-8
0	150	-150
1	122	112
2	26	-19
3	41	-40
4	8	-7
5	38	36
6	50	50
7	29	29
H,L=	1	-9
1	20	-17
2	119	120
3	28	-28
4	24	24
6	44	-43
7	16	-18
H,L=	1	-10
0	110	105
1	21	-20
2	62	58
3	88	83
4	79	-78
5	78	-77
6	24	22
7	14	15
H,L=	1	-11
1	24	23
2	12	-14
3	21	22
4	15	16
5	14	-15
6	2	-1
7	15	16
H,L=	1	-12
0	45	-48
1	37	35
2	34	36
3	46	41
4	27	24
5	37	-38
6	17	-17
H,L=	1	-13
1	29	-29
2	58	57
3	15	-14
4	63	-64
5	14	-13
6	35	-38
H,L=	1	-14
0	32	29
1	38	-34
2	29	-24
3	30	29
4	14	-13
5	10	-8
6	20	21
H,L=	1	-15
1	8	-7
2	63	-63
3	52	50
4	22	20
5	33	34
H,L=	1	-16
0	77	-85
1	38	-44
2	49	-50
3	77	80
4	64	65
5	56	-59
H,L=	1	-17
1	29	30
2	58	63
3	20	-19
4	16	16
H,L=	1	-18
0	87	121
1	36	-47
2	9	-8
3	48	-44
4	17	-14
H,L=	1	-19
1	17	-15
2	47	-43
3	6	7
H,L=	1	-20
0	43	45
1	9	-9
2	56	-56
H,L=	2	-1
1	179	-178
2	179	-176
3	116	119
4	9	9
5	20	22
6	6	-3
7	11	-13
8	22	20
H,L=	2	-2
0	88	84
1	146	-140
2	41	38
3	67	70
4	56	49
5	56	-55
6	7	6
7	20	17
8	27	20
H,L=	2	-3
1	7	-8
2	175	-174
3	53	-50
4	35	34
5	17	-9
6	47	47
7	5	-4
8	16	-14
H,L=	2	-4
0	96	-87
1	147	-145
2	153	-149
3	33	30
4	111	105
5	6	10
6	53	-53
7	25	24
8	10	-9
H,L=	2	-5
1	15	15
2	67	62
3	8	4
4	87	89
5	9	9
6	100	-98
7	7	-8
8	16	15
H,L=	2	-6
0	233	238
1	131	-134
2	54	42
3	109	104
4	31	-31
5	39	-37
6	42	-42
7	18	18
8	49	49
H,L=	2	-7
1	57	-49
2	79	-81
3	18	14
4	34	32
5	10	10
6	13	11
7	27	-26
H,L=	2	-8
0	64	58
1	181	169
2	141	-133
3	35	34
4	135	133
5	45	-40
6	64	-65
7	12	-12
H,L=	2	-9
1	73	69
2	74	69
3	90	-84
4	41	-40
5	29	31
6	84	-88
7	2	0
H,L=	2	-10
0	131	130
1	9	13
2	107	-105
3	33	-31
4	44	44
5	39	39
6	21	22
7	5	1
H,L=	2	-11
1	24	-24
2	13	-14
3	2	-1
4	65	63
5	50	49
6	14	-17
7	35	-36
H,L=	2	-12
0	65	64
1	63	59
2	103	-100
3	11	-7
4	36	30
5	6	-3
6	40	-39
H,L=	2	-13
1	66	64
2	48	-47
3	36	-37
5	19	18
6	11	12
H,L=	2	-14
0	38	36
1	48	49
2	46	-47
3	108	-109
4	61	62
5	66	67
6	8	-5
H,L=	2	-15
1	12	-12
2	39	37
3	8	-6
4	26	26
5	7	8
H,L=	2	-16
0	86	82
1	65	65
2	6	-2
3	59	-59
4	41	-43
5	3	1
H,L=	2	-17
1	19	20
2	53	-51
3	46	-49
4	5	-2
H,L=	2	-18
0	9	11
1	37	34
2	5	-4
3	41	-42
4	42	42
H,L=	2	-19
1	19	-21
2	31	30
3	2	1
H,L=	2	-20
0	7	-9
1	53	54
2	10	13
H,L=	3	-1
1	18	22
2	61	68
3	33	35
4	25	-23
5	34	-32
6	23	-23
7	53	57
8	6	-8
H,L=	3	-2
0	66	65
1	21	-18
2	13	7
3	44	37
4	58	-56
5	57	59
6	37	-37
7	2	-5
8	50	54
H,L=	3	-3
1	91	-86
2	47	-50
3	75	69
4	7	-5
5	49	-46
6	39	41
7	16	-14
8	15	-16
H,L=	3	-4
0	117	-113
1	150	145
2	11	4
3	8	6
4	125	114
5	1	-1
6	46	-45
7	58	-59
8	6	4
H,L=	3	-5
1	53	50
2	156	150
3	88	81
4	15	-15
5	56	-54
6	45	-48
7	15	15
H,L=	3	-6
0	54	-55
1	97	97
2	101	100
3	115	-114
4	56	-52
5	54	57
6	20	-19
7	15	-17
H,L=	3	-7
1	135	-138
2	65	-64
3	47	52
4	32	-37
5	20	21
6	3	-6
7	13	-14
H,L=	3	-8
0	205	-200
1	66	63
2	18	4
3	24	25
4	20	16
5	3	-1
6	50	50
7	43	-48
H,L=	3	-9
1	98	92
2	21	17
3	8	5
4	51	50
5	18	-17
6	12	-12
7	27	29
H,L=	3	-10
0	115	-117
1	18	16
2	83	78
3	115	-114
4	81	-81
5	80	78
6	34	35
7	25	-24
H,L=	3	-11
1	24	-23
2	18	16
3	2	0
4	30	28
6	3	3
7	5	-6
H,L=	3	-12
0	41	38
1	27	27
2	124	123
3	45	-47

TABLE 2. (continued)

K	Fo	Fc	K	Fo	Fc	K	Fo	Fc	K	Fo	Fc	K	Fo	Fc	K	Fo	Fc	K	Fo	Fc	K	Fo	Fc	K	Fo	Fc	K	Fo	Fc
4	125	-125	2	73	-66	4	15	16	2	23	-22	3	14	-15	5	24	-22	2	32	-27	1	23	22	1	31	-51	5	45	42	2	26	-26	2	4	4
5	10	-7	3	29	-26	5	35	-36	3	45	44	4	56	-57	H,L=	5	-16	3	4	5	2	40	-40	2	36	-50	H,L=	8	-2	3	31	30	3	22	-19
6	51	55	4	5	1	6	17	17	H,L=	4	-19	5	6	4	0	19	-20	4	61	58	4	5	-4	3	15	-18	0	84	79	4	7	4	H,L=	9	-9
H,L=	3	-13	5	37	39	7	40	42	1	27	25	6	17	-16	1	45	40	5	8	7	H,L=	6	-16	4	5	6	1	62	-53	H,L=	8	-12	2	28	28
1	44	48	6	18	17	H,L=	4	-10	2	7	-10	7	48	51	2	5	-7	6	3	3	0	91	-110	5	10	10	2	54	-49	0	11	-11	3	25	-24
2	100	-102	7	9	-10	0	62	-58	H,L=	4	-20	H,L=	5	-8	3	50	-48	H,L=	6	-7	1	13	12	6	47	47	3	75	71	1	32	32	H,L=	9	-10
3	79	-82	H,L=	4	-3	1	117	-113	0	48	48	0	99	100	4	22	24	1	67	63	2	43	44	H,L=	7	-8	4	14	-15	2	25	-23	0	6	-4
4	25	28	1	90	-84	2	11	-7	1	44	-45	1	118	110	H,L=	5	-17	2	45	40	3	7	-9	0	68	-70	5	64	-61	3	3	-1	1	31	30
6	6	7	2	7	-3	3	88	87	H,L=	5	-1	2	84	-80	1	12	-12	3	49	-47	H,L=	6	-17	1	75	-71	H,L=	8	-3	H,L=	8	-13	2	13	12
H,L=	3	-14	3	82	78	4	19	16	1	44	-40	3	1	2	2	25	21	4	30	31	2	56	57	2	52	51	1	15	16	1	5	-4	3	39	-32
0	85	-99	4	14	-15	5	28	-30	2	16	-16	4	9	8	3	25	26	5	6	-3	3	8	7	3	32	32	2	62	-57	2	27	30	H,L=	9	-11
1	60	-66	5	36	34	6	7	5	3	28	-24	5	48	50	H,L=	5	-18	6	38	-36	H,L=	6	-18	4	20	21	3	39	-39	3	13	-10	1	6	1
2	72	70	6	32	-36	H,L=	4	-11	5	27	-25	6	10	-10	0	22	22	H,L=	6	-8	0	22	19	5	10	-13	4	10	7	H,L=	8	-14	2	11	12
3	3	0	7	30	-30	1	21	22	6	44	44	H,L=	5	-9	1	46	44	0	6	5	1	4	-6	H,L=	7	-9	5	4	-3	0	14	16	H,L=	9	-12
4	38	-40	H,L=	4	-4	2	60	61	7	25	24	1	15	-13	2	42	43	1	11	10	2	22	18	1	5	-6	H,L=	8	-4	1	4	4	0	4	2
5	49	48	0	63	-60	3	5	-7	H,L=	5	-2	2	2	3	3	33	-32	2	25	-26	H,L=	7	-1	2	20	22	0	59	54	2	21	-19	1	32	32
6	36	36	1	15	-10	4	2	0	0	6	-7	3	14	12	H,L=	5	-19	3	88	-88	1	2	-2	3	9	11	1	126	-118	H,L=	8	-15	2	10	7
H,L=	3	-15	2	19	22	5	33	-35	1	28	-28	4	9	-10	1	8	8	4	34	-34	2	14	14	4	14	-14	2	55	-52	1	11	-11	H,L=	9	-13
1	51	-49	3	108	110	6	47	-49	2	39	-38	5	28	-29	2	40	-39	5	50	54	3	3	-2	5	9	8	3	30	29	2	1	0	1	7	-6
2	17	15	4	21	18	H,L=	4	-12	3	34	-30	6	7	7	H,L=	6	-1	6	6	3	4	27	-27	H,L=	7	-10	4	103	96	H,L=	9	-1	H,L=	10	-1
3	14	11	5	77	-78	0	108	105	4	61	62	H,L=	5	-10	1	7	-11	H,L=	6	-9	5	40	38	0	34	31	5	16	-14	1	15	-12	1	23	23
4	1	1	6	47	47	1	86	-79	5	10	6	0	22	17	2	49	-66	1	46	-42	6	17	16	1	14	-10	H,L=	8	-5	2	10	-5	2	4	5
5	5	5	H,L=	4	-5	2	23	21	6	14	-16	1	103	97	3	14	-15	2	27	-21	H,L=	7	-2	2	15	14	1	33	-28	3	23	-22	H,L=	10	-2
H,L=	3	-16	1	45	43	3	44	40	7	33	33	0	74	-68	5	19	25	3	49	49	0	52	-46	3	49	43	2	24	23	4	21	21	0	30	-30
0	89	-88	2	24	20	4	54	-56	H,L=	5	-3	3	2	-2	6	27	33	4	5	-1	1	19	17	4	54	-48	3	5	6	H,L=	9	-2	1	43	-47
1	59	59	3	19	17	6	3	2	1	4	-2	4	72	66	H,L=	6	-2	5	31	27	2	35	34	5	4	0	4	6	-4	0	53	52	2	45	47
2	94	95	4	9	9	H,L=	4	-13	2	19	17	5	7	4	0	36	66	6	13	8	3	55	53	H,L=	9	-11	5	16	17	1	4	0	H,L=	10	-3
3	42	38	5	61	-62	1	46	-42	3	56	59	6	20	-20	1	7	4	H,L=	6	-10	4	43	-44	1	29	1	H,L=	8	-6	2	14	-15	1	15	-19
4	97	-97	6	33	35	2	82	-83	4	12	-9	H,L=	5	-11	2	26	-21	0	26	-21	5	15	-12	2	43	12	0	102	109	3	40	-43	2	20	-25
5	2	0	7	31	32	3	30	27	5	25	26	1	74	72	3	15	14	1	115	114	6	47	47	H,L=	7	-12	1	33	-37	4	3	1	H,L=	10	-4
H,L=	3	-17	H,L=	4	-6	4	21	22	6	7	-6	2	49	48	4	85	81	2	51	44	H,L=	7	-3	0	35	-33	2	73	-73	H,L=	9	-3	0	62	-83
1	55	52	0	142	-138	5	22	23	H,L=	5	-4	3	11	10	5	8	-11	3	60	-57	1	7	7	1	52	-51	3	53	51	1	15	-18	1	9	-12
2	5	-2	1	18	-16	6	14	15	0	59	81	4	15	7	6	33	-35	4	27	-27	2	20	16	2	21	25	4	102	95	2	56	-34	2	29	41
3	5	-3	2	12	-4	H,L=	4	-14	1	8	-11	5	19	-21	7	26	-25	5	20	19	3	18	-17	3	18	15	5	18	-17	3	34	33	H,L=	10	-5
4	10	10	3	85	-83	0	88	-85	2	22	-26	6	11	-13	H,L=	6	-3	6	44	46	4	6	4	4	5	-2	H,L=	8	-7	4	6	4	2	2	-4
H,L=	3	-18	4	13	3	1	67	-70	3	43	54	H,L=	5	-12	1	29	23	H,L=	6	-11	5	15	-12	H,L=	7	-13	1	9	6	H,L=	9	-4	H,L=	10	-6
0	74	-72	5	16	15	2	43	-41	4	11	-14	0	79	76	2	39	41	1	34	34	H,L=	7	-4	1	10	8	2	29	-33	0	11	16	0	58	-57
1	37	-32	6	11	-11	3	142	143	5	26	-29	1	13	12	3	46	-47	2	44	-42	0	108	-102	2	21	17	3	14	17	1	56	79	1	60	-57
2	39	38	7	41	42	4	54	54	6	16	-19	2	64	-66	4	12	-10	3	62	-62	1	12	-7	3	4	1	4	14	-14	2	12	-13	2	54	49
3	20	21	H,L=	4	-7	5	60	-59	7	7	8	3	108	-102	5	33	-32	4	23	24	2	59	55	4	13	-12	5	16	-16	3	3	-5	H,L=	10	-7
4	20	-20	1	43	-42	H,L=	4	-15	H,L=	5	-5	4	20	19	6	34	-33	5	17	-17	3	10	9	H,L=	7	-14	H,L=	8	-8	4	12	16	1	27	-23
H,L=	3	-19	2	92	92	1	67	66	1	16	26	5	59	56	7	29	31	H,L=	6	-12	4	28	-24	0	26	25	0	23	31	H,L=	9	-5	2	19	17
1	9	-3	3	60	62	2	19	19	2	6	-11	6	44	-47	H,L=	6	-4	0	54	-46	5	10	6	2	32	-34	1	4	-2	1	37	55	H,L=	10	-8
2	5	5	4	32	-36	3	7	-7	3	39	-32	H,L=	5	-13	0	66	66	1	37	-40	6	23	22	3	9	9	2	35	-39	2	1	-1	0	22	20
3	18	-18	5	21	22	4	26	27	4	11	13	1	87	-81	1	59	56	2	17	13	H,L=	7	-5	4	7	8	3	17	17	3	39	-37	1	23	-20
H,L=	3	-20	6	6	-5	5	22	-22	5	61	-68	2	57	-54	2	41	-39	3	79	-75	1	23	24	H,L=	7	-15	4	58	66	4	9	-3	2	5	-4
0	32	-31	7	13	-15	H,L=	4	-16	6	22	23	3	69	66	3	62	-59	4	7	9	2	42	42	1	33	-36	5	15	-20	H,L=	9	-6	H,L=	10	-9
1	55	-54	H,L=	4	-8	0	44	45	7	7	8	4	13	9	4	47	-48	5	54	52	3	52	49	2	6	6	H,L=	8	-9	0	24	20	1	17	15
2	30	30	0	139	172	1	112	-114	H,L=	5	-6	5	14	-16	5	91	91	H,L=	6	-13	4	24	-31	3	4	4	1	14	20	1	6	-5	H,L=	10	-10
H,L=	4	-1	1	35	-44	2	19	-22	0	180	167	H,L=	5	-14	6	8	-7	1	52	-49	5	12	-11	H,L=	7	-16	2	45	46	2	43	-38	0	8	-13
1	13	12	2	44	49	3	19	-14	1	0	-7	0	82	-77	H,L=	6	-5	2	16	13	6	15	15	0	14	-14	3	19	-19	3	84	-75			
2	56	54	3	59	70	4	25	25	2	56	-49	1	75	72	1	12	-9	3	34	36	H,L=	7	-6	1	45	48	4	16	-16	4	13	10			
3	21	-21	4	66	-73	H,L=	4	-17	3	56	-49	2	39	37	2	35	-37	4	3	5	0	39	-48	2	13	-12	H,L=	8	-10	H,L=	9	-7			
4	40	-38	5	78	-98	1	68	-63	4	59	57	3	69	-70	3	24	25	5	31	32	1	28	-26	H,L=	7	-17	0	110	108	1	43	-40			
5	9	-7	6	19	22	2	27	-28	5	41	-41	4	42	40	4	4	-3	H,L=	6	-14	2	53	58	1	34	40	1	15	-18	2	12	10			
6	7	4	7	13	14	3	39	37	6	54	-55	5	22	24	5	19	16	1	71	71	3	6	-14	2	31	-33	H,L=	8	-1	2	102	-98	3	48	
7	22	20	H,L=	4	-9	4	17	16	7	30	29	H,L=	5	-15	6	17	20	2	72	67	4	62	-67	1	24	-19	3	4	0	4	4	0			
H,L=	4	-2	1	7	10	H,L=	4	-18	H,L=	5	-7	1	14	-17	H,L=	6	-6	3	14	11	5	33	-34	2	30	29	4	30	29	H,L=	9	-8			
0	8	-12	2	113	-104	0	4	-4	1	24	-18	3	23	23	0	9	-5	4	76	-73	6	26	30	3	13	10	H,L=	8	-11	0	27	-22			
1	16	10	3	75	-69	1	11	-16	2	21	23	4	6	-3	1	102	93	H,L=	6	-15	H,L=	7	-7	4	15	12	1	15	-16	1	113	105			

a) Six reflections, 021, 022, 210, 204, 214, and 244, were excluded from the least-squares refinement probably because of the high extinction effect.

the International Tables for X-Ray Crystallography.[8]

Results and Discussion

The final atomic parameters are given in Table 3, together with their estimated standard deviations. As shown in Fig. 1, there are two molecules (A and B) in an asymmetric unit and one hydrogen atom of a sulfonate group is protonated to the nitrogen atom of a guanidyl group. Thus, the two molecules of GGPSA occur in zwitterionic forms, $(NH_2)_2{}^+CNHCH_2CH_2CH_2SO_3{}^-$, as in the case of GGBOPSA,[6] L-arginine dihydrate,[7] γ-aminobutyric acid (GABA),[9] γ-amino-β-hydroxybutyric acid (GABOB),[10] taurine,[11,12] homotaurine[13] and γ-guanidinobutyric acid hydrochloride (GGBA·HCl).[14]

Bond Distances and Angles. The interatomic distances and angles are listed in Table 4 together with their standard deviations. The bond lengths and angles of the two molecules are similar and acceptable as a whole. However, the length for C(A2)–(A3) (1.523 Å) is shorter than that for C(B2)–C(B3) (1.552 Å), which may be due to the difference in C(3)–N(1) distance.

In the sulfonate group, the averages of three S–O distances, three O–S–O angles and three O–S–C(1) angles are 1.457 Å, 112.3° and 106.5° (molecule A) and 1.456 Å, 112.4° and 106.3° (molecule B), respectively. These values are very similar to those of other compounds containing a sulfonate group; GGBOPSA,[6] taurine[11,12] and homotariune.[13] The deviations of angles around the sulfur atom from tetrahedral angles are probably due to the van der Waals repulsion by the short contacts of O–O distances which are averaged to be 2.42 Å in both molecules as in the case of GGBOPSA.[6]

In the guanidyl group, the three C–N distances of

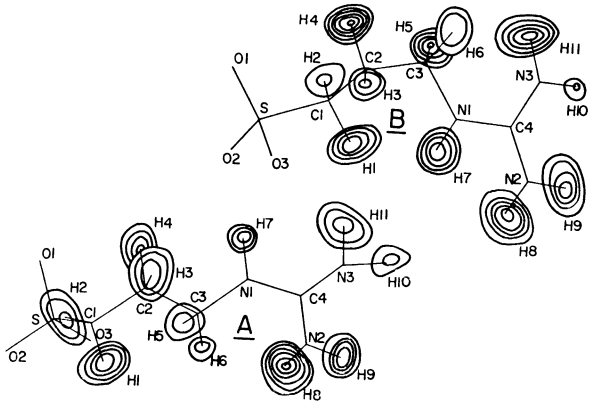

Fig. 1. Difference Fourier map of GGPSA. Contours are drawn at intervals of 0.1 e.Å^{-3}, starting with the contour of 0.3 e.Å^{-3}.

8) "International Tables for X-Ray Crystallography," Vol. 3, Kynoch Press, England (1962).

9) K. Tomita, T. Fujiwara, and H. Higashi, *Jap. J. Brain Physiol.*, **111**, 111 (1971).

10) K. Tomita, M. Harada, and T. Fujiwara, This Bulletin, to be published.

11) H. H. Sutherland and D. W. Young, *Acta Crystallogr.*, **16**, 897 (1963).

12) Y. Okaya, *ibid.*, **21**, 726 (1966).

13) S. Ueoka, T. Fujiwara, and K. Tomita, This Bulletin, **45**, 3634 (1972).

14) T. Maeda, T. Fujiwara, and K. Tomita, *ibid.*, **45**, 3628 (1972).

Table 3. Final positional and thermal parameters (estimated standard deviations in parentheses)
Anisotropic temperature factors are expressed in the form
$\exp\{-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk + B_{13}hl + B_{23}kl)\}$.

Atom	x	y	z	B_{11} or B	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
S (A)	0.6591 (2)	0.2493 (2)	0.0329 (1)	0.0050 (2)	0.0094 (3)	0.0009 (1)	0.0015 (4)	0.0013 (2)	0.0001 (2)
O (A1)	0.5224 (5)	0.2271 (7)	−0.0002 (3)	0.0055 (5)	0.0170 (10)	0.0018 (2)	−0.0015 (12)	−0.0012 (4)	−0.0014 (6)
O (A2)	0.7518 (5)	0.2695 (7)	−0.0175 (2)	0.0071 (5)	0.0189 (10)	0.0011 (2)	0.0003 (12)	0.0029 (4)	−0.0004 (6)
O (A3)	0.7043 (5)	0.1203 (6)	0.0828 (3)	0.0117 (7)	0.0106 (9)	0.0016 (2)	0.0089 (12)	0.0031 (5)	0.0021 (6)
C (A1)	0.6671 (8)	0.4430 (9)	0.0771 (4)	0.0132 (10)	0.0082 (12)	0.0015 (2)	−0.0006 (18)	0.0030 (7)	0.0003 (8)
C (A2)	0.5716 (8)	0.4550 (10)	0.1312 (4)	0.0109 (9)	0.0132 (14)	0.0014 (2)	0.0012 (19)	0.0023 (7)	−0.0000 (9)
C (A3)	0.6286 (7)	0.3759 (10)	0.1993 (4)	0.0089 (9)	0.0169 (15)	0.0015 (2)	0.0045 (19)	0.0033 (7)	0.0016 (9)
C (A4)	0.5682 (7)	0.3673 (9)	0.3170 (4)	0.0063 (8)	0.0100 (12)	0.0018 (2)	−0.0018 (16)	0.0009 (6)	−0.0002 (8)
N (A1)	0.5354 (6)	0.4008 (8)	0.2490 (3)	0.0090 (8)	0.0153 (12)	0.0012 (2)	0.0028 (15)	0.0014 (6)	0.0011 (7)
N (A2)	0.6806 (6)	0.2876 (8)	0.3387 (3)	0.0089 (7)	0.0152 (12)	0.0007 (2)	0.0064 (15)	0.0010 (5)	−0.0009 (7)
N (A3)	0.4878 (7)	0.4198 (8)	0.3591 (3)	0.0116 (8)	0.0159 (12)	0.0017 (2)	0.0073 (17)	0.0045 (6)	−0.0004 (8)
S (B)	0.1650 (2)	0.3698 (3)	0.2202 (1)	0.0073 (2)	0.0117 (3)	0.0008 (1)	−0.0026 (4)	0.0012 (2)	−0.0003 (2)
O (B1)	0.0457 (5)	0.4103 (7)	0.1738 (3)	0.0101 (6)	0.0180 (11)	0.0012 (2)	0.0059 (13)	−0.0003 (5)	−0.0010 (6)
O (B2)	0.2479 (5)	0.2401 (7)	0.1940 (3)	0.0109 (7)	0.0213 (12)	0.0014 (2)	0.0078 (14)	0.0038 (5)	−0.0014 (7)
O (B3)	0.2469 (6)	0.5144 (7)	0.2426 (3)	0.0143 (7)	0.0150 (10)	0.0018 (2)	−0.0145 (14)	0.0023 (5)	0.0001 (7)
C (B1)	0.1172 (7)	0.2847 (9)	0.2967 (3)	0.0085 (8)	0.0109 (12)	0.0010 (2)	−0.0009 (16)	0.0030 (6)	0.0001 (8)
C (B2)	0.0264 (7)	0.4057 (9)	0.3294 (3)	0.0074 (8)	0.0120 (13)	0.0012 (2)	−0.0013 (16)	0.0023 (6)	0.0007 (8)
C (B3)	0.0023 (7)	0.3407 (9)	0.4008 (3)	0.0071 (8)	0.0117 (13)	0.0013 (2)	−0.0016 (16)	0.0012 (6)	0.0014 (8)
C (B4)	0.1391 (7)	0.2976 (8)	0.5124 (4)	0.0072 (8)	0.0095 (12)	0.0015 (2)	−0.0034 (15)	0.0026 (6)	−0.0003 (8)
N (B1)	0.1261 (5)	0.3517 (7)	0.4472 (3)	0.0068 (6)	0.0115 (10)	0.0011 (2)	−0.0024 (13)	0.0007 (5)	0.0009 (7)
N (B2)	0.2571 (6)	0.3107 (8)	0.5516 (3)	0.0066 (7)	0.0205 (13)	0.0010 (2)	−0.0030 (15)	0.0012 (5)	0.0013 (8)
N (B3)	0.0357 (6)	0.2282 (8)	0.5360 (3)	0.0072 (7)	0.0168 (12)	0.0013 (2)	−0.0055 (15)	0.0014 (5)	0.0037 (7)
H (A1)	0.761	0.456	0.103	1.612					
H (A2)	0.647	0.530	0.043	3.878					
H (A3)	0.560	0.566	0.139	4.052					
H (A4)	0.481	0.419	0.113	1.778					
H (A5)	0.660	0.252	0.187	4.183					
H (A6)	0.713	0.443	0.212	3.959					
H (A7)	0.454	0.446	0.236	2.049					
H (A8)	0.713	0.211	0.312	2.159					
H (A9)	0.700	0.274	0.380	1.990					
H (A10)	0.480	0.405	0.405	5.576					
H (A11)	0.392	0.485	0.348	5.346					
H (B1)	0.207	0.256	0.329	1.327					
H (B2)	0.055	0.145	0.284	8.076					
H (B3)	0.067	0.517	0.339	3.020					
H (B4)	−0.063	0.420	0.301	1.953					
H (B5)	−0.025	0.220	0.401	1.972					
H (B6)	−0.079	0.428	0.416	3.804					
H (B7)	0.209	0.431	0.437	1.958					
H (B8)	0.338	0.329	0.539	2.543					
H (B9)	0.266	0.299	0.591	3.230					
H (B10)	0.042	0.174	0.582	2.719					
H (B11)	−0.061	0.229	0.523	3.543					

Table 4. Bond lengths (Å) and angles (°) of GGPSA (estimated standard deviations listed in parentheses)

	A	B		A	B
S-O(1)	1.449(5)	1.441(5)	O(1)-S-O(2)	111.4(3)	113.6(4)
S-O(2)	1.466(5)	1.472(6)	O(1)-S-O(3)	113.8(3)	113.6(4)
S-O(3)	1.455(5)	1.455(6)	O(2)-S-O(3)	111.6(3)	110.0(4)
S-C(1)	1.777(8)	1.781(7)	C(1)-S-O(1)	107.6(4)	108.8(4)
C(1)-C(2)	1.538(11)	1.537(9)	C(1)-S-O(2)	104.3(4)	105.2(4)
C(2)-C(3)	1.523(11)	1.552(10)	C(1)-S-O(3)	107.5(4)	105.0(4)
C(3)-N(1)	1.464(10)	1.443(9)	S-C(1)-C(2)	113.9(6)	111.3(5)
C(4)-N(1)	1.360(9)	1.345(8)	C(1)-C(2)-C(3)	113.0(7)	110.4(6)
C(4)-N(2)	1.318(9)	1.327(9)	C(2)-C(3)-N(1)	109.7(6)	108.8(6)
C(4)-N(3)	1.310(9)	1.323(9)	C(3)-N(1)-C(4)	122.9(6)	123.1(6)
			N(1)-C(4)-N(2)	119.6(7)	119.3(6)
			N(1)-C(4)-N(3)	118.4(7)	119.8(6)
			N(2)-C(4)-N(3)	122.0(7)	120.9(7)

each molecule have normal values. Separations of the guanidyl group from the backbone, *i. e.*, C(3)–N(1) distance, are 1.464 Å (A) and 1.443 Å (B), and are very similar to those of GGBOPSA (1.456 Å), γ-guanidinobutyric acid hydrochloride (GGBA·HCl) (1.477 Å[14]) and L-arginine dihydrate (1.471 Å[7]). The three N–C(4)–N angles are 119.6°, 122.0° and 122.0 118.4° (A) and 119.3°, 120.9° and 119.8° (B). C(4)–N distances are averaged to be 1.329 Å and 1.332 Å for A and B, respectively, indicating to that they have somewhat double bond character. 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 approximately 24%, 37%, and 39% for A, and 29%, 35%, and 36% for B, whereas the corresponding values for GGBOPSA[6] and GGBA·HCl[14] are 32%, 25%, and 43%, and 35%, 29%, and 36%, respectively.

The C–H and N–H distances are within the ranges 0.91 Å—1.29 Å and 0.77 Å—1.09 Å, respectively.

Conformation. Conformations of the two molecules are of great interest, those around C(1)–C(2) and C(2)–C(3) being *gauche-trans* in molecule A, and *trans-gauche* in molecule B (Fig. 2). GGBOPSA,[6] GABA·HCl,[9] GABOB,[10] homotaurine[13] and GGBA·HCl[14] showed *trans-trans* conformations, and GABA[16] a *gauche-trans* form similar to molecule A. The *trans-gauche* conformation of molecule B, however, is a rare one in the derivatives of γ-amino acid and γ-guanidino acid so far investigated. Conformations of the sulfonate group around S–C(1), took the most stabilized forms (Fig. 2).

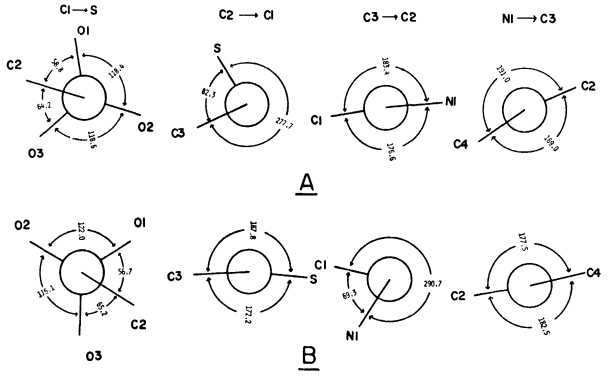

Fig. 2. Newman projection of atoms around four bonds. The arrow indicates the bond direction viewing down from front to back of paper.

The torsion angles around C(3)–N(1) are 169.0° (A) and 177.5° (B), which mean roughly a *trans* conformation similar to that of GGBOPSA[6] and L-arginine dihydrate.[7]

Planarity. The guanidyl groups are essentially planar in both molecules. Equations of the least-squares plane of each molecule through the atoms N(1)–C(4)–N(2)–N(3) and deviations of individual atoms from the corresponding plane are listed in Table 5. The planarity of guanidyl groups in GGPSA is in good agreement with that of GGBOPSA,[6] L-arginine dihydrate[7] and of GGBA·HCl.[14]

The dihedral angles between the plane of a guanidyl group and that passing through C(1)–C(2)–C(3) are 12.95° in molecule A, and 69.87° in molecule B. The corresponding angle of GGBOPSA is 27.4°. Molecule A therefore, has a value nearer that of GGBOPSA, since both have *trans zigzag* conformations.

Crystal Structure. Distances and angles of hydrogen bonds are listed in Table 6. All feasible hydrogen atoms in the molecule are utilized to form hydrogen bonds, the molecules being held together by a three-dimensional network of NH···O hydrogen bonds (Fig. 3).

In molecule A, the guanidyl group is connected with five neighboring molecules by seven hydrogen bonds and the sulfonate group performs the role as an acceptor of six hydrogen bonds. The distances of N(Al) to O(B2) and to O(B3) are 3.215 Å and 3.033 Å, respectively, and the N(Al)–H(A7) bond is directed to bisect these two directions. The distances of N(A3) to O(B3) of the original molecule and to O(A3) of a neighboring molecule translated by operation of (x, $0.5-y$, $0.5+z$) are 3.188 Å and 2.876 Å, respectively, the N(A3)–H(A11) bond bisecting the two directions. Thus, the H(A7) and H(A11) atoms are considered to contribute to form bifurcated hydrogen bonds.

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

16) K. Tomita, H. Higashi, and T. Fujiwara, This Bulletin, **46**, 2199 (1973).

Table 5. Equations of least-squares planes and deviations of individual atoms from the planes of guanidyl groups in GGPSA

	Equations[a)]	Deviations of atoms in Å			
		N (1)	C (4)	N (2)	N (3)
GGPSA (A)	$-0.48255X-0.86818Y-0.11577Z=-5.61564$	−0.0028	+0.0089	−0.0031	−0.0030
GGPSA (B)	$0.31393X-0.89952Y-0.30382Z=-5.18435$	+0.0031	−0.0093	+0.0031	+0.0031

a) X, Y, and Z are orthogonal coordinates in Å parallel to a, b, and c^*.

Table 6. Hydrogen bond lengths and angles of GGPSA

Bond lengths		Bond angles	
N (A1)-H (A7)·····O (B2) (I)	3.215 Å	C (A3)-N (A1)-O (B2) (I)	110.7°
N (A1)-H (A7)·····O (B3) (I)	3.033 Å	C (A4)-N (A1)-O (B2) (I)	109.5°
N (A2)-H (A8)·····O (B3) (II)	2.869 Å	C (A3)-N (A1)-O (B3) (I)	135.7°
N (A2)-H (A9)·····O (A2) (III)	2.861 Å	C (A4)-N (A1)-O (B3) (I)	101.4°
N (A3)-H (A10) ···O (A1) (III)	2.987 Å	C (A4)-N (A2)-O (B3) (II)	117.6°
N (A3)-H (A11) ···O (A3) (IV)	2.876 Å	C (A4)-N (A2)-O (A2) (III)	118.9°
N (A3)-H (A11) ···O (B3) (I)	3.188 Å	C (A4)-N (A3)-O (A1) (III)	139.6°
		C (A4)-N (A3)-O (B3) (I)	95.5°
		C (A4)-N (A3)-O (A3) (IV)	160.8°
N (B1)-H (B7)·····O (A3) (IV)	2.862 Å	C (B3)-N (B1)-O (A3) (IV)	113.8°
N (B2)-H (B8)·····O (A1) (III)	3.011 Å	C (B4)-N (B1)-O (A3) (IV)	117.4°
N (B2)-H (B9)·····O (B2) (III)	2.852 Å	C (B4)-N (B2)-O (A1) (III)	124.1°
N (B3)-H (B10) ···O (B1) (III)	2.922 Å	C (B4)-N (B2)-O (B2) (III)	114.2°
N (B3)-H (B11) ···O (A2) (V)	2.906 Å	C (B4)-N (B3)-O (B1) (III)	124.2°
		C (B4)-N (B3)-O (A2) (V)	130.8°

(I) (x, y, z); (II) $(x, -0.5-y, 0.5+z)$; (III) $(x, 0.5-y, -0.5+z)$; (IV) $(x, 0.5-y, 0.5+z)$; (V) $(-1+x, 0.5-y, -0.5+z)$

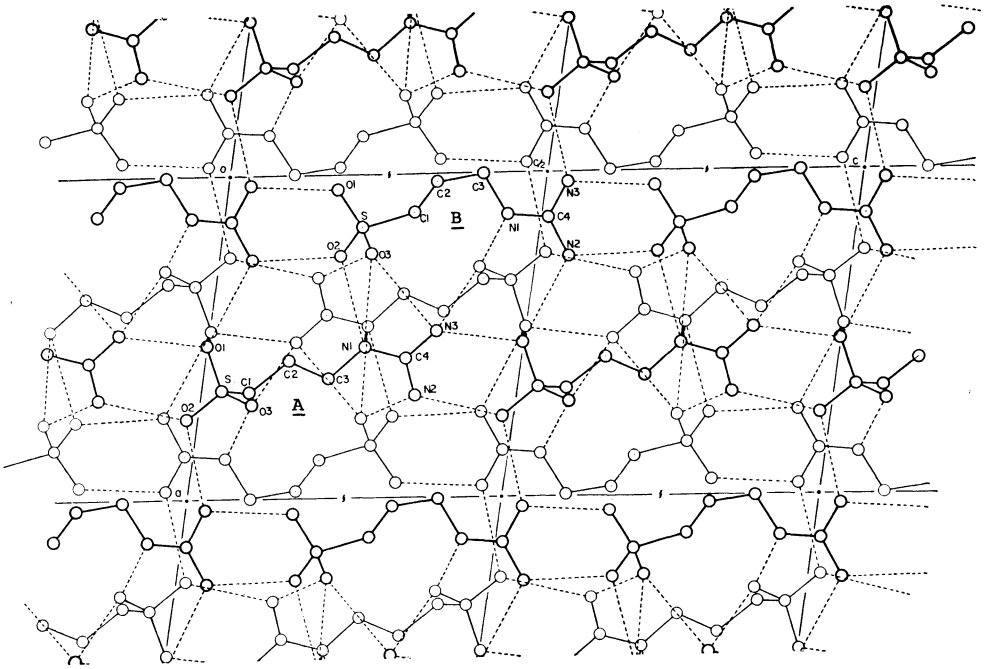

Fig. 3. The crystal structure projected along b-axis.

In molecule B, the guanidyl group is connected with four neighboring molecules by five hydrogen bonds, the sulfonate group fulfilling the role as an acceptor of six hydrogen bonds.

On the other hand, the guanidyl group of GGBO-PSA[6] is connected with three neighboring molecules by six hydrogen bonds, and the sulfonate group performs the role of an acceptor of five hydrogen bonds and the N(2)–H bond is bifurcated to O(2) and O(4) of (2-x, 1-y, 1-z).

Homotaurine molecules are jointed to each other with three NH···O hydrogen bonds to form a three-dimensional network, and there are three NH···O intermolecular and one intramolecular hydrogen bonds in taurine.

The intermolecular contacts between adjacemt molecules are kept by normal van der Waals distances.

We wish to thank Prof. S. Tsunoo and Dr. K. Horisaka, Showa Medical School, for valuable adivce and for supply of the sample. This work was partly supported by a research grant from the Ministry of Education.