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MOLECULAR STRUCTURE OF γ-GUANIDINO-β-HYDROXY PROPANE SULFONIC ACID DETERMINED BY X-RAY METHOD

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The molecular structure of γ-guanidino-β-hydroxy propane sulfonic acid was determined by X-ray diffraction method and we described some structural features compared with other related compounds.

ω-Amino acids act as chemical transmitter in the central nervous system and we have deep interests in the relations between molecular structure and function of ω-amino acids, ω-amino sulfonic acids and their derivatives. Some structural features of ω-amino acids and their derivatives were reported previously[1]. This communication presents briefly the molecular structure of γ-guanidino-β-hydroxy propane sulfonic acid (GGBOPSA) and discussion of some structural similarities between related compounds.

The crystal and molecular structure of GGBOPSA has been determined by X-ray method. A sample of this compound was recrystallized from aqueous solution as transparent prism-shaped crystals. The cell constants were determined from the Weissenberg and precession photographs. The density was measured by flotation method in the mixture of ethylene dibromide and carbon tetrachloride. The crystal data of GGBOPSA are shown in Table 1 with those of related compounds. The intensities of reflections collected around a-axis were estimated visually and the structure was solved by the usual heavy-atom method. The refinement of structure is now in progress by using the block diagonal least-squares procedure. Figure 1 shows the superimposed electron density map to (010) plane at the stage of R value 0.15.

Table 1. CRYSTAL DATA

Compounds	GGBOPSA	GGPSA*)	GGBOBA**)
Chemical Formula	$C_4H_{11}O_4N_3S$	$C_4H_{10}O_3N_3S$	$C_5H_{11}O_3N_3$
Molecular Weight	197.21	181.20	161.16
Crystal System	Monoclinic	Monoclinic	Triclinic
Space Group	$P2_1/c$	$P2_1/c$	$P\bar{1}$
a (Å)	7.44	10.080	8.46
b (Å)	9.89	8.013	9.89
c (Å)	11.11	19.716	4.86
α (°)	90	90	91.9
β (°)	97.7	98.17	111.6
γ (°)	90	90	70.3
Volume (Å^3)	810.2	1576.32	355.75
$D_{obs.}$ (g.cm^{-3})	1.621	1.518	1.494
$D_{calc.}$ (g.cm^{-3})	1.617	1.522	1.504
Z	4	8	2

*) GGPSA : γ-guanidino propane sulfonic acid

**) GGBOBA: γ-guanidino-β-hydroxy butyric acid

The structure determination of these compounds is now in progress in our laboratory.

The bond lengths and angles had reasonable values compared with those of other compounds such as L-arginine[2], taurine[3,4], homotaurine[5], γ-amino butyric acid[6], γ-amino-β-hydroxy butyric acid (GABOB)[7] and γ-guanidino butyric acid HCl[8] : similarly with the case of taurine and homotaurine, three S-O bonds of the SO_3 group are in the state of resonance. The guanidyl group is planar and one C4-N3 bond is slightly shorter than the other two C-N distances. It may be due to the difference in double bond character or the difference in the intermolecular hydrogen bonds.

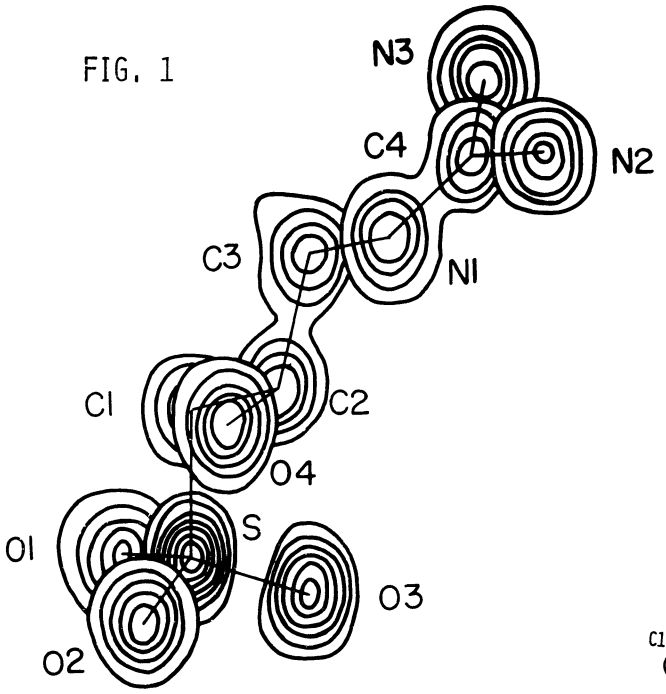
Being protonated one hydrogen atom of SO_3H group to the nitrogen of guanidyl group, GGBOPSA occurs in zwitterionic form in crystalline state. The existence of this hydrogen atom was confirmed by the difference Fourier synthesis. Though the physiological actions of GGBOPSA are still unknown, the skeletal conformation of this molecule (C1-C2-C3-N1) is planar trans zigzag form as seen

in GABOB which has a potent physiological action in central nervous system[9] and we suppose that this rigidity of molecular backbone is substantial for understanding the mechanism of drug action.

As shown in Figure 2, d- and l-forms of GGBOPSA were dimerized through the NH---O hydrogen bond related by center of symmetry. The view of the packing, projected downward the c-axis is shown in Figure 3. Among the hydrogen atoms in the molecule, all feasible hydrogen atoms are utilized to form hydrogen bonds and the molecules are closely packed in the crystal, being fixed through three dimensional net work of hydrogen bonds.

Further details of the structure will be published elsewhere in the near future.

FIG. 1



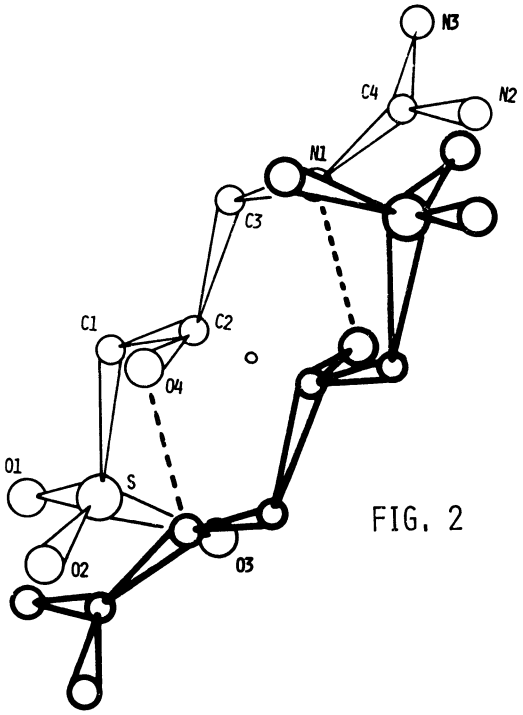
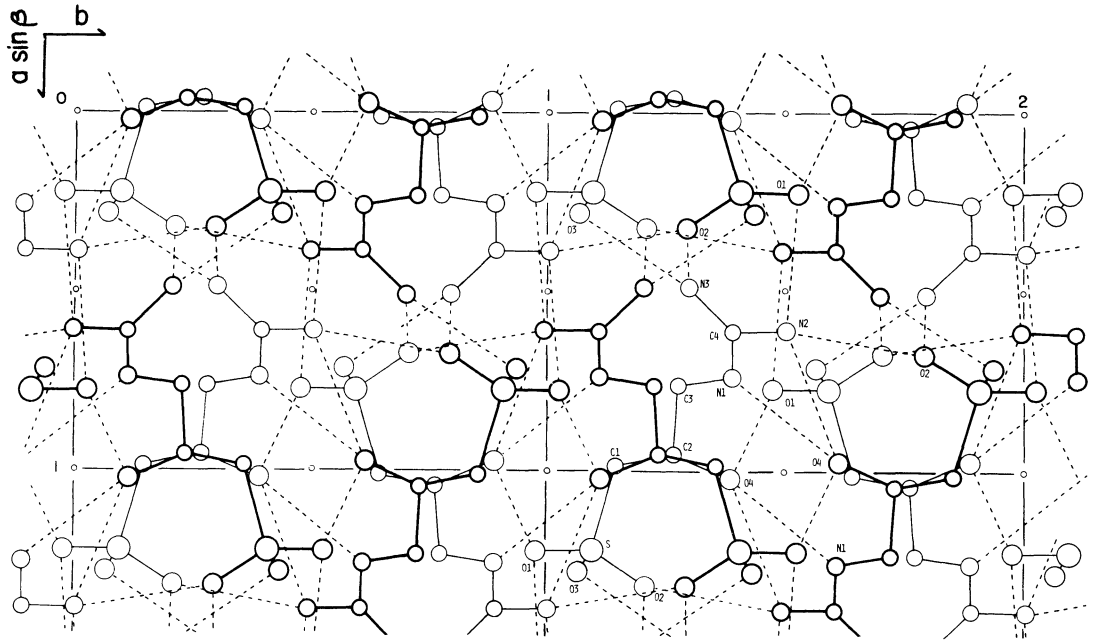


FIG. 2

FIG. 3



References

1) K.Tomita, Tetrahedron Letters, 27, 2587(1971)

2) I.L.Karle and J.Karle, Acta Cryst., 17, 835(1964)

3) H.H.Sutherland and D.W.Young, Acta Cryst., 16, 897(1963)

4) Y.Okaya, Acta Cryst., 21, 726(1966)

5) S.Ueoka, T.Fujiwara, and K.Tomita, to be published

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

7) M.Harada, H.Higashi, T.Fujiwara, and K.Tomita, unpublished results

8) T.Maeda, T.Fujiwara, and K.Tomita, to be published

9) T.Hayashi and K.Nagai, Proc. 20th Int. Physiol. Cong., p.410(1951)

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