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CRYSTAL DATA AND SOME STRUCTURAL FEATURES OF γ-AMINOBUTYRIC ACID, 3-AMINOPROPANE SULFONIC ACID AND THEIR DERIVATIVES

Ken-ichi Tomita

Faculty of Pharmaceutical Sciences, Osaka University

Toneyama, Toyonaka, Osaka, Japan

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It is well known that the proteins consist of over twenty α-amino acids. However, many ω-amino acids or ω-amino sulfonic acids have been isolated from various sources of the animals and plants.

Numerous investigations have been pointed to accumulate data as to the metabolic pathway or the knowledge of physiological functions of these particular compounds, and it has been shown that the certain ω-amino acids or ω-amino sulfonic acids strongly influence the behaviour of neurones when applied extracellularly. One of the most important results was that γ-aminobutyric acid and γ-amino-β-hydroxybutyric acid originally synthesized by M.Tomita[1] were found to have a potent inhibitory action against epileptic seizure[2].

It is of most interest to investigate systematically the molecular structure of such important compounds, and elucidate the relation of the molecular conformation to its specific physiological action. Since 1965, the author and collaborators have been deeply interesting about such substantial points, and Table 1 presents the crystal data of γ-aminobutyric acid, 3-aminopropane sulfonic acid and their derivatives so far investigated by X-rays in this laboratory.

It was found that there are some common features about the molecular structure of these compounds as follows. 1) Molecule is the so-called zwitterionic in the crystalline state as in α-amino acids. 2) Molecule has the planar carbon skeletal conformation in crystal of the compounds so far investigated except γ-aminobutyric acid. On the other hand, no one has such planar conformation in glycine[3], β-alanine[4], ε-aminocapronic acid[5] and taurine[6]. 3) Molecule

except γ-aminocrotonic acid and γ-aminobutyric acid has trans-zigzag skeletal configuration including the amino-nitrogen and carboxyl-carbon atoms in γ-amino acids or the amino-nitrogen and sulfonyl-sulfur atoms in γ-amino sulfonic acids.

The detailed crystal structure analysis of each compound is now in progress and will be published elsewhere in the near future.

Table 1

COMPOUND*1)	DENSITY ($g.cm^{-3}$)	CRYSTAL SYSTEM	SPACE GROUP	z	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	INTENSITY DATA*2)	STRUCTURE DETERMINATION
GABA	1.226	monoclinic	$P2_1/c$	4	7.18	10.18	8.26	90.0	111.4	90.0	F	determined [7]
GABA HCl	1.362	monoclinic	$P2_1$	2	5.93	6.54	9.09	90.0	100.0	90.0	F	determined [8]
GABOB	1.459	monoclinic	$P2_1/c$	4	7.43	8.29	9.34	90.0	110.9	90.0	F	determined [7]
GACA HBr	1.830	monoclinic	$P2_1$	2	7.82	6.51	6.67	90.0	104.0	90.0	F	determined [9]
GGBA HBr	1.664	triclinic	$P\bar{1}$	2	7.94	9.36	7.78	103.2	115.5	61.5	F	determined [10]
GGBA HCl	1.429	triclinic	$P\bar{1}$	2	7.41	9.12	7.25	101.5	112.4	65.2	F	determined [10]
GAPSA(α)	1.610	orthorhombic	$Pmn2_1$	2	7.06	5.49	7.43	90.0	90.0	90.0	C	determined [11]
GAPSA(β)	1.599	orthorhombic	$P2_12_12_1$	4	14.12	5.50	7.43	90.0	90.0	90.0	F	in progress
GABOPSA	1.686	orthorhombic	Pbca	8	9.91	12.03	10.25	90.0	90.0	90.0	C	in progress

*1) Abbreviations: GABA, γ-aminobutyric acid; GABOB, γ-amino-β-hydroxybutyric acid; GACA, γ-aminocrotonic acid; GGBA, γ-guanidinobutyric acid; GAPSA, 3-aminopropane sulfonic acid (homotaurine); GABOPSA, 3-amino-2-hydroxypropane sulfonic acid;

*2) Intensity data were collected by film (F) or counter (C) method.

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