Presented at the *Third National Symposium on Graduate Research* held at
Suranaree University of Technology, Nakhon Ratchasima, Thailand, 18-19 July 2002.

Title: Crystal and Molecular Structure of the Beta Form of L-Glutamic Acid

Author: Nongnaphat Khosavithitkul and Kenneth J. Haller
Presenter: Nongnaphat Khosavithitkul
Organization: School of Chemistry
Institute of Science
Suranaree University of Technology
Nakhon Ratchasima 30000
E-mail/phone: unchalee@ccs.sut.ac.th (044)224-757
Session: Science-Engineering-Technology

The single crystal x-ray structure of L-glutamic acid was first reported based on photographic data by S. Hirokawa (*Acta Cryst., 8*, 637, 1955). The low resolution study was carried out at room temperature and resulted in a relatively high discrepancy index, R = 15.0%. A neutron diffraction study was carried out in 1972 (M. S. Lehmann, T. F. Koetzle, W. C. Hamilton, *J. Cryst. Mol. Struc., 2*, 225, 1972).

One carboxylic acid proton has transferred to the nitrogen atom giving a zwitterion in the solid state. The C-C and C-N intramolecular bond distances are unremarkable. The anionic carboxylate C-O bonds are unequal, 1.2488(10) and 1.2636(10) Å. The shorter C-O bond is to the oxygen atom that participates in the strongest intermolecular hydrogen bond (2.518(1) Å to the carboxylic acid hydrogen of an adjacent molecule). The C-O bonds of the carboxylic acid group are normal at d[C-O] = 1.3145(11) and d[C=O] = 1.2197(11) Å.

One hydrogen atom on the cationic nitrogen participates in a strong intramolecular hydrogen bond to a carboxylate oxygen (2.477(1) Å and a strong intermolecular hydrogen bond to the other carboxylate oxygen (2.871(1) of an adjacent molecule. The other two hydrogen atoms on the nitrogen also participate in strong intermolecular hydrogen bonds (2.859(1) and 2.912(1) Å).

Recrystallized from water as transparent colorless hexagonal needles. *Crystal Data:* $C_5H_9NO_4$, MW = 147.14 Daltons, orthorhombic, $P2_12_12_1$ (No. 19), a = 5.1480(1), b = 6.9171(1), c = 17.2801(3) Å, V = 613.33(2) Å^3, T = 200±1 K, z = 4, d_{calc} = 1.588 Mg m^{-3}, μ = 0.09 mm^{-1}, MoKα radiation (λ = 0.71073 Å), F_{000} = 312., $sin\theta/\lambda_{max}$ = 0.61 Å^{-1}, R_{int} = 0.037, 2827 unique data, 2591 Fo>4σ(Fo), R_1 = 0.0342, wR_2 = 0.0857, gof = 1.074, ρ_{max} = 0.30(6) e A^{-3}.