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Micro-Raman studies on the conformational behaviors of monosodium glutamate in dehydration process

Jing Jing Shou, Guang Zeng, Hao Zhang, Yun Hong Zhang *

The Institute of Chemical Physics, Key Laboratory of Cluster Science, Beijing Institute of Technology, Beijing 100081, China

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Abstract

The conformational behaviors of monosodium glutamate (MSG) in a dehydration process were studied by Micro-Raman spectroscopy in combination with Hartree–Fock calculations using 6-31+G* method. The dehydration process of the MSG droplet was performed by decreasing the ambient relative humidity (RH). The intensity ratio of the 935 cm^{-1} band to 884 cm^{-1} band (I_{935}/I_{884}) kept decreasing when RH decreased. By optimizing the geometries with different fixed dihedral angles, the downtrend of (I_{935}/I_{884}) is found to be due to the reduction of MSG molecular volume.

Keywords: Raman; MSG; Calculation; Dehydration; Intensity; Dihedral angle

The conformational behavior of amino acids and their vibrational characteristics are important. The intrinsic conformational properties and energies determine to a large extent the functional specificity of proteins and polypeptides [1]. Biological systems are usually associated with aqueous solutions, where solute–solvent interactions significantly influence the energy, structure and vibrations of the amino acids [2].

Glutamate is an α-amino which can be easily found in protein-containing foods. Monosodium glutamate (MSG) known as a flavor enhancer is a zwitterionic structure of glutamate [3]. MSG is one of the most abundant excitatory neurotransmitters in higher life forms. It has a particular interest to current models of memory and learning [4]. It has been proved that excessive MSG can cause damages to the brains of young rodents [5]. Most previous investigations on the MSG molecule are based on theoretical calculations which might be different from the real condition [6,7]. Recently, infrared and Raman spectroscopy were imported on this subject [8,9]. But few investigations were carried out to study the MSG at high concentration or colloidal state. In present work, the conformation change of MSG in dehydration process was studied by Micro-Raman spectroscopy in combination with theoretical calculation.

1. Experimental

MSG was dissolved into triply distilled water by 1.0 mol/L. The pH of the solution was 6.8. A MSG droplet (∼100 μm in diameter) was injected onto a quartz substrate by a syringe. Then the quartz substrate was fixed on the

* Corresponding author.
E-mail address: yhz@bit.edu.cn (Y.H. Zhang).

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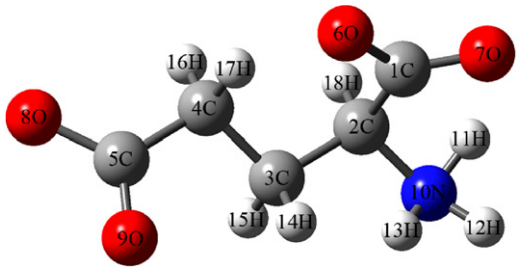

Fig. 1. Structure of MSG molecule with the atomic numbering used in this work.

bottom of a chamber sealed with thin transparent polyethylene (PE) film. The chamber was mounted on an automated motorized stage. The RH in the chamber was adjusted discretely by adjusting the flow ratio of water-saturated N_2 and dry N_2. The RH and temperature of the gas fed into the chamber were measured by a humidity temperature meter with the accuracy of $\pm 2.5\%$ and ± 0.7 K.

Raman spectra were obtained by the Raman microscope (Renishaw Invia) with a 514.5 nm argon ion laser. The data were recorded under the following conditions: laser power, 20 mW; number of scan, 20; exposure time, 10 s and spectral resolution, 1 cm^{-1}. To make the droplet completely equilibrate with a given ambient RH, 40 min was spent before each Raman measurement. All the measurements were made at ambient temperature of 293 K.

Both geometrical optimizations and vibrational frequency calculations were performed at HF/6-31+G* level by using Gaussian 03 program. All calculations were carried out with default convergence criteria of Gaussian 03 program. There are three main dihedral angles deciding the framework of MSG. They are illustrated in Fig. 1 as C_1–C_2–C_3–C_4, C_2–C_3–C_4–C_5 and N–C_2–C_3–C_4, which are defined as θ, φ and ω for simplicity. For comparison, vibrational frequency calculations were performed with fixed θ or φ from 0° to 180° with a step of 10° while the other variables were fully optimized.

2. Results and discussion

The saturated RH of the monosodium glutamate solution measured is about $90 \pm 2\%$. Crystallization was not observed in the MSG droplets even at the lowest RH. Raman spectroscopy can provide exquisite molecular details of

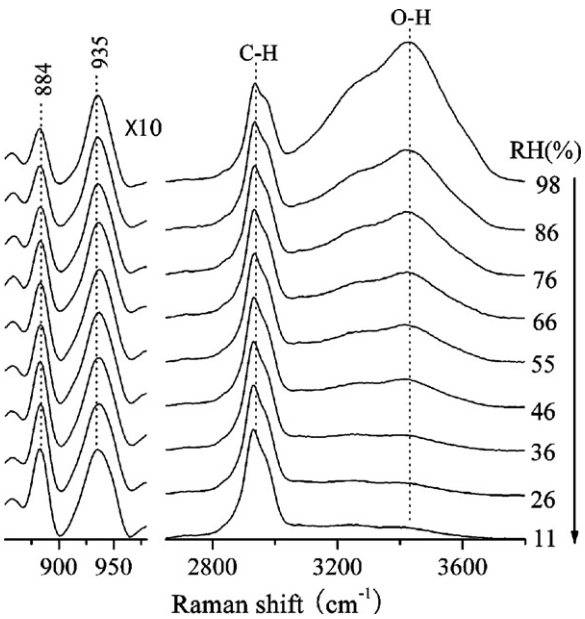

Fig. 2. Raman spectra of MSG droplet at various RH values.