Cold Ion Spectroscopy of Host-Guest Complexes in the Gas Phase

Yoshiya Inokuchi

Department of Chemistry, Graduate School of Sciences, Hiroshima University, Kagamiyama 1-3-1, Higashi-Hiroshima, Hiroshima 739-8526, Japan y-inokuchi@hiroshima-u.ac.jp

"Cold" ion spectroscopy in the gas phase is a powerful method to reveal conformational landscapes of complicated systems such as biological species [1]. Electronic transition energy is quite sensitive to the conformation, which can be separately observed for different conformers thanks to the cooling of ions by using a cold, 22-pole ion trap. Resolved electronic transitions enable us to measure infrared spectra by infrared-ultraviolet double-resonance and to determine the structure and the number of the conformers. In 2010, we started our first collaboration project between the EPFL (École Polytechnique Fédérale de Lausanne) and Hiroshima University. Since then, we have applied this method to host-guest systems containing benzo-crown ethers and metal ions [2–6]. In this talk, we will present the results of the benzo-crown ether-metal ion complexes, and discuss the relation between the ion selectivity of the crown ethers and their conformation under bare and micro-solvated conditions.

References

- Boyarkin, O. V.; Mercier, S. R.; Kamariotis, A.; Rizzo, T. R., "Electronic Spectroscopy of Cold, Protonated Tryptophan and Tyrosine", *J. Am. Chem. Soc.* 2006, 128, 2816-2817.
- [2] Inokuchi, Y.; Boyarkin, O. V.; Kusaka, R.; Haino, T.; Ebata, T.; Rizzo, T. R., "UV and IR Spectroscopic Studies of Cold Alkali Metal Ion-Crown Ether Complexes in the Gas Phase", J. Am. Chem. Soc. 2011, 133, 12256-12263.
- [3] Inokuchi, Y.; Boyarkin, O. V.; Kusaka, R.; Haino, T.; Ebata, T.; Rizzo, T. R., "Ion Selectivity of Crown Ethers Investigated by UV and IR Spectroscopy in a Cold Ion Trap", J. Phys. Chem. A 2012, 116, 4057-4068.
- [4] Inokuchi, Y.; Boyarkin, O. V.; Ebata, T.; Rizzo, T. R., "UV and IR Spectroscopy of Cold 1,2-Dimethoxybenzene Complexes with Alkali Metal Ions", *Phys. Chem. Chem. Phys.* **2012**, *14*, 4457-4462.
- [5] Inokuchi, Y.; Kusaka, R.; Ebata, T.; Boyarkin, O. V.; Rizzo, T. R., "Laser Spectroscopic Study of Cold Host-Guest Complexes of Crown Ethers in the Gas Phase", *ChemPhysChem* 2013, 14, 649-660.
- [6] Inokuchi, Y.; Ebata, T.; Rizzo; T. R. Boyarkin, O. V. "Microhydration Effects on the Encapsulation of Potassium Ion by Dibenzo-18-Crown-6", J. Am. Chem. Soc. 2014, 136, 1815-1824.