Spectroscopic Studies on Host-Guest Complexes in the Gas Phase and on Gold Surface

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

Host molecules such as crown ethers show the selective capture of guest species. Despite their wide use such as phase transfer catalysts in organic synthesis, the origin of their functionality has not been fully understood at the molecular level; our final goal is to reveal the origin of the guest selectivity in solution by spectroscopic methods. For this purpose, we have been using two methods. One is laser spectroscopy of cold host-guest complexes in the gas phase, using supersonic jet expansion or a cold ion trap.¹⁻⁴ The other is surface-enhanced infrared absorption spectroscopy (SEIRAS) of the complexes tagged on gold surface.⁵ In the former, we produce cold host-guest complexes in vacuum and apply laser-based methods such as laser-induced fluorescence, resonance-enhanced multiphoton ionization, IR-UV double-resonance, UV-UV hole-burning, and UV photodissociation. In the latter, we prepare thiol (-SH) derivatives of host molecules by organic synthesis and bind them on gold surface through gold-sulfur (Au-S) bond. Solutions containing guest species are put on the surface, inducing the complex formation between the tagged hosts and the guests, and the complexes can be detected by SEIRS. In this talk we will present our recent progress in these techniques, mainly on complexes holding cation guests.

References

- Y. Inokuchi et al., "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.
- [2] Y. Inokuchi et al., "Ion Selectivity of Crown Ethers Investigated by UV and IR Spectroscopy in a Cold Ion Trap", J. Phys. Chem. A 2012, 116, 4057-4068.
- [3] Y. Inokuchi et al., "Laser Spectroscopic Study of Cold Host-Guest Complexes of Crown Ethers in the Gas Phase", *ChemPhysChem* **2013**, *14*, 649-660.
- [4] Y. Inokuchi et al., "Microhydration Effects on the Encapsulation of Potassium Ion by Dibenzo-18-Crown-6", J. Am. Chem. Soc. 2014, 136, 1815-1824.
- [5] Y. Inokuchi et al., "Formation of Host-Guest Complexes on Gold Surface Investigated by Surface-Enhanced IR Absorption Spectroscopy", *Chem. Phys. Lett.* **2014**, *592*, 90-95.