

UV and IR Spectroscopy of Host-Guest Complexes in a Cold Ion Trap

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Host molecules such as crown ethers and calixarenes show the selective capture of guest species. Despite their wide use such as phase transfer catalysts or building blocks of supramolecular compounds in organic chemistry, 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 inclusion by spectroscopic methods. In this study, we construct a new mass spectrometer equipped with an electrospray ionization (ESI) and a cold, quadrupole Paul ion trap (Fig. 1).

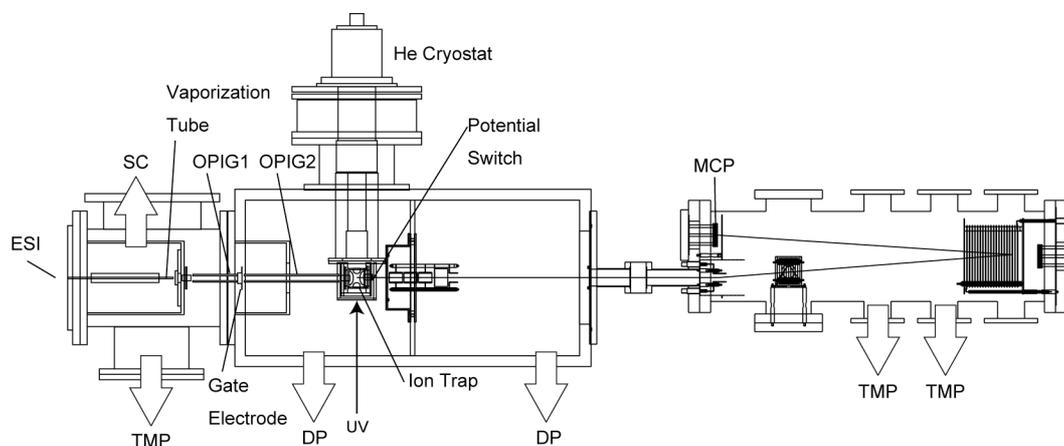


Figure 1. Schematic drawing of a mass spectrometer used in this study.

Ion complexes are produced by the ESI and led into the Paul ion trap, which is cooled down to ~ 4 K by a He cryostat. He buffer gas is introduced into the trap, and the ion complexes are cooled by the collision with the cold He gas. The ion complexes are irradiated by a UV laser, and resulting fragment ions are mass-analyzed by a time-of-flight mass spectrometer. UV photodissociation (UVPD) spectra of the ion complexes are obtained by plotting the yield of the fragment ions against UV wavenumber. Figure 2 shows UVPD spectra of $K^+\cdot(\text{benzo-18-crown-6})$ complex. In previous studies, it has been considered that ions cannot be cooled below ~ 30 K using the Paul trap (Fig. 2b). By taking a great care to the cooling efficiency, however, we can obtain cold ions (~ 10 K) even using the Paul trap (Fig. 2c). In this study, we examine the complex structure of cold benzo-crown ethers and calix[4]arene complexes with alkali metal ions on the basis of UV and IR spectra, and discuss on the relation between the structure and the ion selectivity [1, 2].

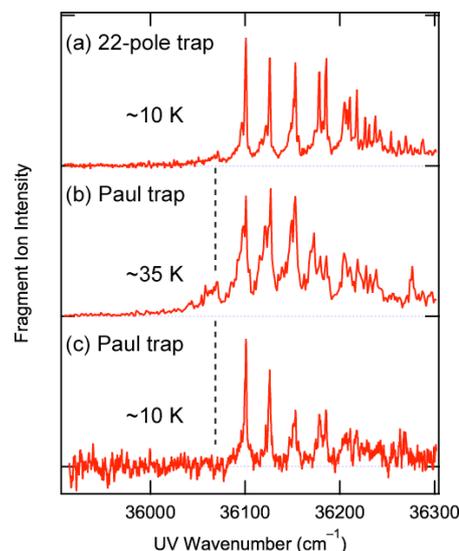


Figure 2. UVPD spectra of $K^+\cdot B18C6$

[1] Inokuchi et al., *J. Am. Chem. Soc.*, **136**, 1815 (2014).

[2] Inokuchi et al., *J. Am. Chem. Soc.*, **133**, 12256 (2011).