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

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Introduction

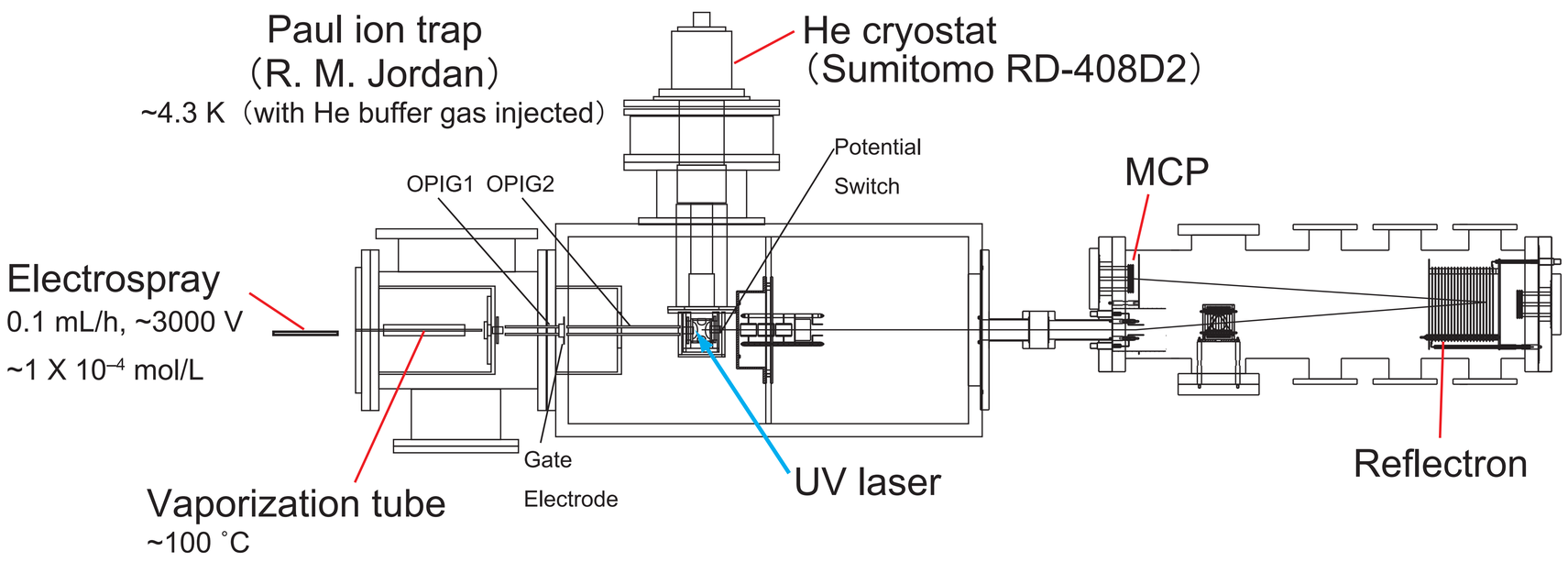
■The purpose of this study is to examine the structure of ion complexes for functional molecules spectroscopically under cold conditions in the gas phase, and to reveal the relation between the structure and their functions.

■We construct a time-of-flight mass spectrometer for UV photodissociation spectroscopy, equipped with an electrospray ion source and a cold quadrupole Paul ion trap.

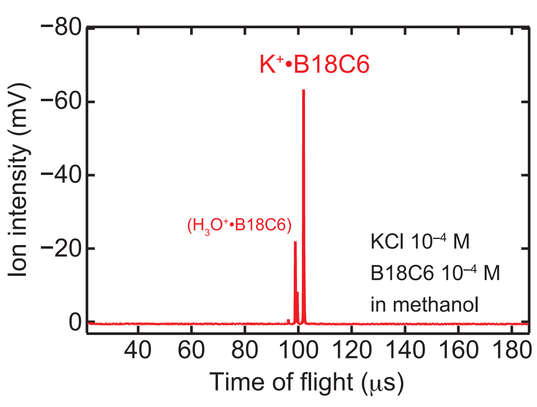
■We achieve ~10 K of the ion (vibrational) temperature with a cold Paul ion trap, which is cooler than that in previous studies (~30 K) and shows a drastic change on the UV spectrum.

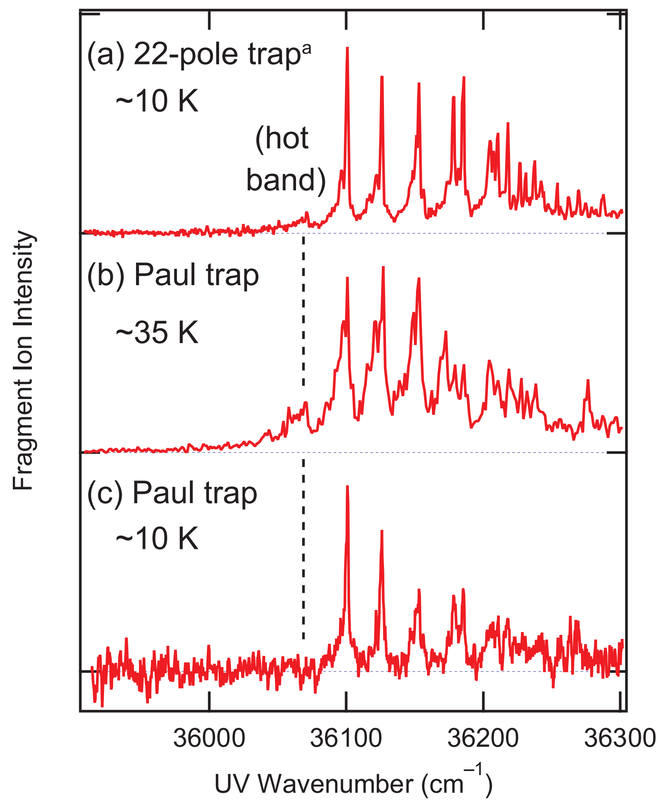
■We demonstrate the application of our apparatus to ion complexes of benzo-18-crown-6 (B18C6) and calix[4]arene (C4A) with alkali metal ions.

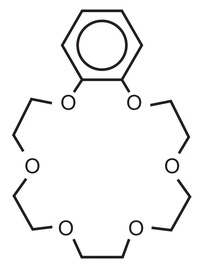
Mass spectrometer for UV photodissociation (UVPD) spectroscopy



K^+•B18C6 complex







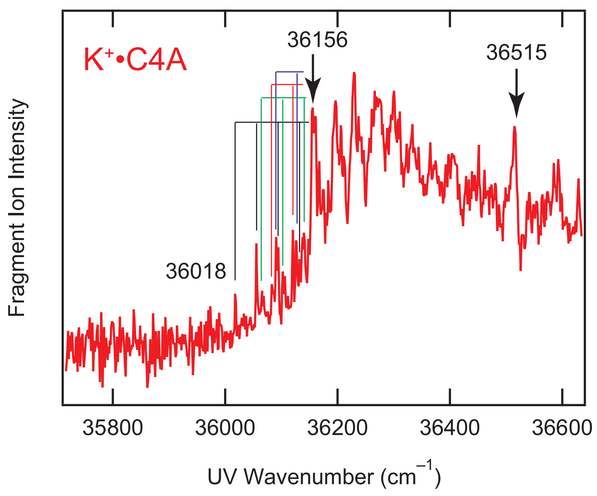
benzo-18-crown-6
(B18C6)

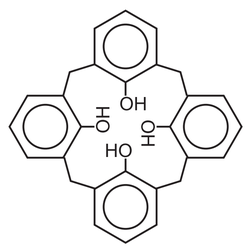
One problem to cool ions with a Paul ion trap was insufficient cooling of tapped ions (up to ~30 K).

→ Finally we achieve ~10 K with the Paul trap by optimizing trapping conditions.

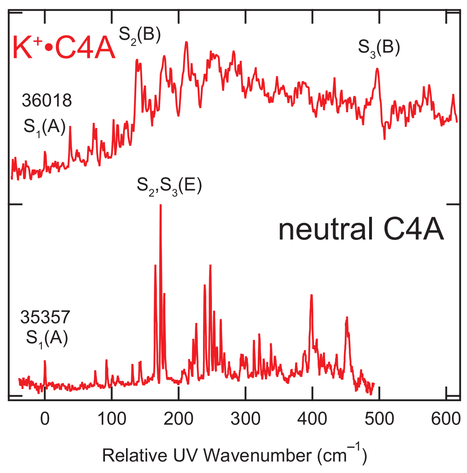
[a]Inokuchi et al., JPCA, 2012, 116, 4057.

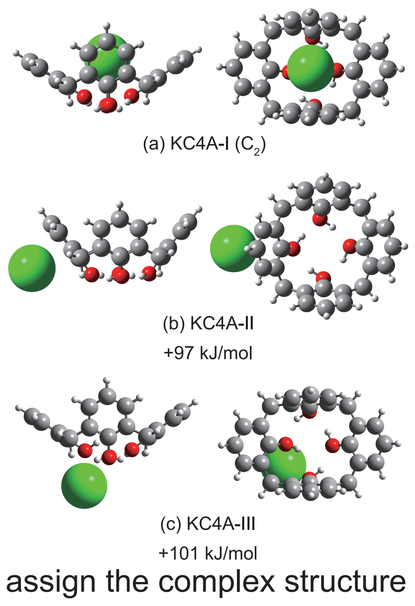
K^+•C4A complexes[b]





Calix[4]arene
(C4A)





A weak, sharp (1.8 cm^{-1}) band is observed at 36018 cm^{-1}, followed by a strong one at 36156 cm^{-1}.

Similarity of the UV spectra between bare C4A (C_4 symmetry)[c] and K^+•C4A suggests that a high symmetry is kept for K^+•C4A upon complexation with K^+.

We assign the complex structure of K^+•C4A to KC4A-I (C_2 symmetry) on the basis of DFT and TD-DFT results at M05-2X/6-31+G(d).

[b]Inokuchi et al., submitted to JPCA. [c]Ebata et al., JCP, 2007, 126, 141101.

■We will apply our instrument to a number of host-guest complexes such as crown ethers, calix-arenes, calixresorcinarenes, and cyclodextrines.