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The geometric and electronic structures of dibenzo-15-crown-5 complexes with alkali metal ions studied by cold ion trap-laser spectroscopy

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Crown ethers (CEs) have been widely used as host molecules in host-guest, supramolecular, and organic chemistry. In this study, we examine the geometric and electronic structures of dibenzo-15-crown-5 (DB15C5) complexes with alkali metal ions, $M^+ \cdot \text{DB15C5}$ ($M = \text{Li, Na, K, Rb, and Cs}$), by UV photodissociation (UVPD) and UV-UV hole-burning (HB) spectroscopy under cold (~ 10 K) conditions in the gas phase.

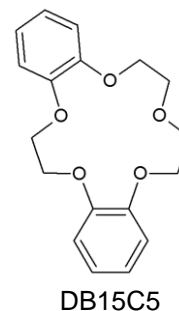


Figure 1 displays the UVPD spectra of the $M^+ \cdot \text{DB15C5}$ ($M = \text{Li, Na, K, Rb, and Cs}$) complexes in the $36000\text{--}37500\text{ cm}^{-1}$ region. The UVPD spectrum of the $\text{K}^+ \cdot \text{DB15C5}$ complex (Fig. 1c) has an extensive and intense progression in the $36600\text{--}36800\text{ cm}^{-1}$ region, but with no strong origin band. In addition to this progression, a strong band also appears at 36839 cm^{-1} , followed by a progression of several vibronic bands. Since the interval and intensity pattern are different between these two progressions, these can be ascribed to different isomers or different electronic states. Figure 2 shows the UV-UV HB spectra with the UVPD spectra for the $\text{K}^+ \cdot \text{DB15C5}$ complex. All the vibronic bands, which include the extensive progression on the lower frequency side, appear in the UV-UV HB spectra. This results indicate that all the vibronic bands appearing in the $36600\text{--}37000\text{ cm}^{-1}$ region are due to a single isomer.

In this talk, we will determine the geometric and electronic structures of the $M^+ \cdot \text{DB15C5}$, and discuss the difference between the $M^+ \cdot \text{DB15C5}$, $M^+ \cdot \text{B15C5}$, and $M^+ \cdot \text{DB18C6}$ complexes.

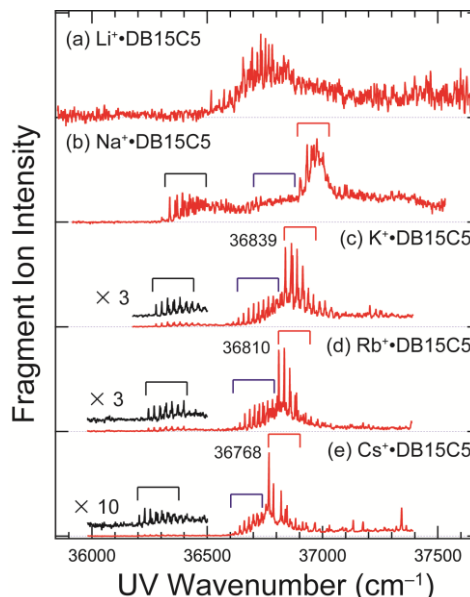


Fig. 1 UVPD spectra of the $M^+ \cdot \text{DB15C5}$

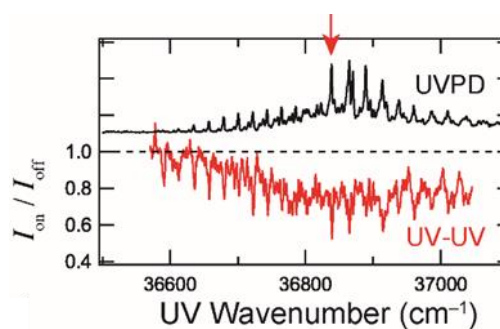


Fig. 2 UV-UV HB spectra for the $\text{K}^+ \cdot \text{DB15C5}$