CONFORMATION-SPECIFIC INFRARED AND ULTRAVIOLET SPECTROSCOPY OF DIBENZO-15-CROWN-5-$(H_2O)_1$-CLUSTER: RESHAPING A BINDING POCKET

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Crown ethers are oxygen containing macrocycles noted for their ability to preferentially bind substrates such as ions and water. Despite the high symmetry inherent to the chemical structure, crown ethers are remarkably flexible, adapting their conformation to the substrate to which they are bound. Here, we present the conformational preferences of the singly hydrated dibenzo-15-crown-5 ether (DB15C) complex formed and cooled in a supersonic jet. The resonance enhanced two-photon ionization, UV-UV holeburning, and resonant ion-dip infrared spectra lead to the identification of a single DB15C-$(H_2O)_1$ conformer with the water doubly hydrogen bonded to the crown. Single vibronic level dispersed fluorescence identified both electronic origins and the coupling between the two chromophores. Finally, infrared population transfer spectroscopy is used to study the monomer conformer populations formed by infrared photodissocation of the complex via the water OH stretch transitions, providing unique insight to the energy flow between water and crown.