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ENCAPSULATION OF WATER MOLECULES BY DIBENZO-18-CROWN-6-ETHER IN A SUPERSONIC JET

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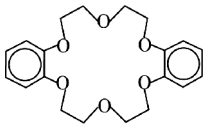
Introduction Crown ethers are well known host molecules which encapsulate cations selectively and efficiently. Crown ethers can also encapsulate variety of neutral molecules such as water and biomolecules. In order to elucidate the mechanism and structures of encapsulation of guest molecules in the crown cavity, we choose water as a guest and investigate the hydrated structures of dibenzo-18-crown-6-ether (DB18C6) by using supersonic jet and laser spectroscopy.



DB18C6

Experiments The supersonic jet of DB18C6 was obtained by an adiabatic expansion of gaseous DB18C6 mixed with He carrier gas into vacuum. Its hydrated clusters were obtained by using water/He premixed carrier gas. The electronic and IR spectra for those species were obtained by laser induced fluorescence (LIF), UV-UV hole-burning (HB), and IR-UV double-resonance spectroscopy.

Results and Discussion Fig. 1(a) shows LIF spectrum of DB18C6 and its hydrated clusters. Since the LIF spectrum shows complicated feature, we measure HB spectra in Fig. 1(b)-(h) by monitoring the labeled bands (**m1**, **m2**, **a**, **c**–**e**). As the results, we distinguish eight different species. The bands **m1** and **m2** are due to different conformers of bare DB18C6, while the bands **a**-**f** are due to DB18C6-$(H_2O)_n$. Fig. 2(a)-(c) show the IR-UV double-resonance spectra of the bands **a**-**c** in the region of OH stretching vibrations. Since the spectra of bands **a** and **b** exhibit two OH bands at slightly different position, the species **a** and **b** are assigned to the different isomers of DB18C6-$(H_2O)_1$. From the frequencies and intensities of the OH stretch bands, the water molecules are thought to be hydrogen-bonded with bidentate form in these species. The IR-UV spectrum of band **c** exhibits four bands, indicating that the species **c** is DB18C6-$(H_2O)_2$. Most probable structures calculated at B3LYP/6-31+G* are also shown in Fig. 2. In the presentation, we will discuss the structures of DB18C6-$(H_2O)_n$ with n = 1-4 in more detail.

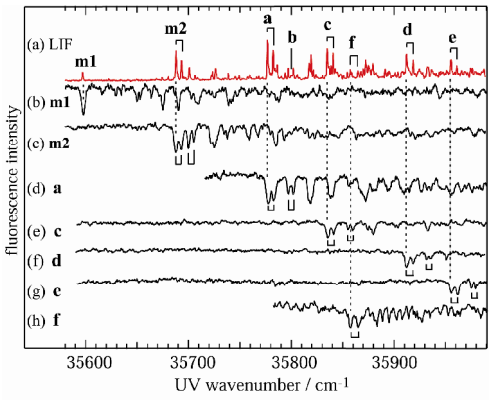


Fig. 1 (a) LIF and (b)-(h) UV-UV hole-burning spectra

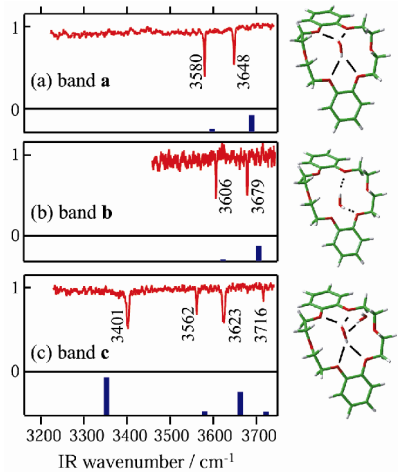


Fig. 2 IR-UV double-reasonance spectra, optimized structures, and IR spectra calculated (B3LYP/6-31+G*)