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Water-mediated conformer optimization in benzo-18-crown-6-ether/water system

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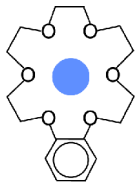
[Introduction] Crown ethers (CEs) are known as functional molecules which can encapsulate various guest species in their cavity. The key point for the efficient encapsulation is whether size and shape of guest species fit into the cavity of CEs. In the present work, we investigated conformation of benzo-18-crown-6-ether (B18C6) and structures of B18C6-$(H_2O)_n$ clusters under a jet-cooled condition. We report that B18C6 adjusts its conformation to encapsulate water molecules efficiently.


B18C6

[Experimental] The jet-cooled B18C6 was obtained by an adiabatic expansion of gaseous B18C6 mixed with helium carrier gas in the vacuum chamber. B18C6-$(H_2O)_n$ clusters were obtained by the expansion of B18C6 with water vapor/helium premixed carrier gas. The electronic and IR spectra of those species were obtained by laser induced fluorescence (LIF) and IR-UV double-resonance spectroscopy, respectively. The obtained spectra were analyzed with an aid of quantum chemical calculations.

[Results] Fig. 1 shows S_1-S_0 LIF spectrum of jet-cooled B18C6-$(H_2O)_{0\text{-}4}$. The bands labeled by **M1**-**M4** are the different conformers of bare B18C6. Bands **A**-**D** are due to B18C6-$(H_2O)_1$, bands **E**-**G** to B18C6-$(H_2O)_2$, band **H** to B18C6-$(H_2O)_3$, and band **I** to B18C6-$(H_2O)_4$. As shown in the scheme in Fig. 1, the number of conformers in bare form (**M1**-**M4**) decreases to mostly one conformer upon the complexation with a water molecule (species **D**). Water hydrogen bond networks in species **E**-**I** are grown based on species **D**. The details of experimental and calculated results will be discussed.

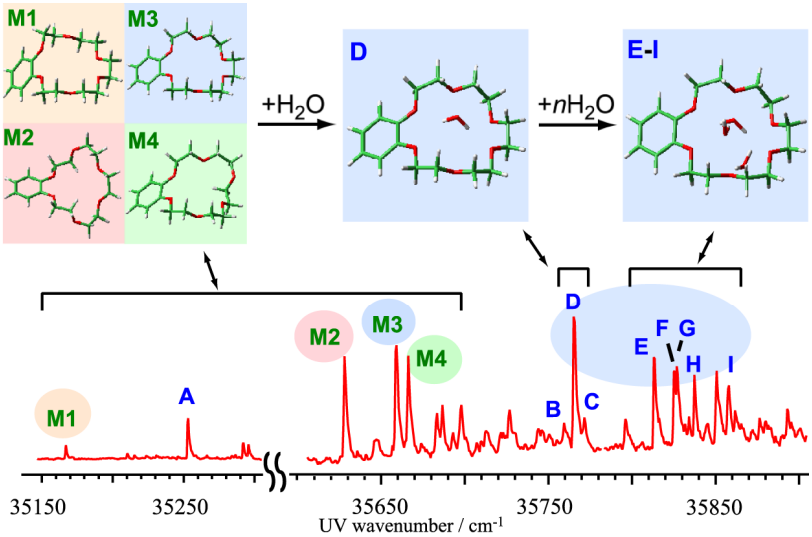


Fig. 1 LIF spectrum of B18C6-$(H_2O)_{0\text{-}4}$ and a scheme of "water-mediated conformer optimization in B18C6/water system".