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

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UV and IR spectra of jet-cooled Dibenzo-18-crown-6-ether (DB18C6) and DB18C6-$(H_2O)_n$ are observed by laser induced fluorescence (LIF), UV-UV hole-burning and IR-UV double resonance spectroscopy [a]. The LIF spectrum exhibited complicated vibronic structure in the region of 35500-36800 cm^{-1}. The UV-UV hole-burning and IR-UV double resonance spectra suggest the existence of two conformers for DB18C6; one is "boat-type" structure having C_2v symmetry, and the other is "chair-type" structure having C_i symmetry. For the hydrated clusters, we assigned most of them to the "boat-type" DB18C6-$(H_2O)_{n=1-4}$. Details of the encapsulation structure in DB18C6-$(H_2O)_{n=1-4}$ will be discussed by the comparison of the observed IR spectra with those obtained by quantum chemical calculation.

[a] R. Kusaka, Y. Inokuchi, and T. Ebata, Phys. Chem. Chem. Phys. 9, 4452 (2007).