1E1a

Laser spectroscopic study of β-estradiol and its hydrated clusters in a supersonic jet

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Introduction: 17β-estradiol(E_2) is the most active endogenous estrogen and it is a main female hormone that comprises a group of compounds, including estrone, estradiol, and estriol. Estrogens exert their several physiological effects by binding to the estrogen receptors. The key point of the physiological activity of estrogen is hydrogen(H)-bonding ability of A-ring and D-ring OH. Here, we have investigated the structure of bare E_2 and its 1:1 hydrated clusters by using supersonic jets and various laser spectroscopic methods. We discuss the conformation of E_2 and the H-bonded structure.

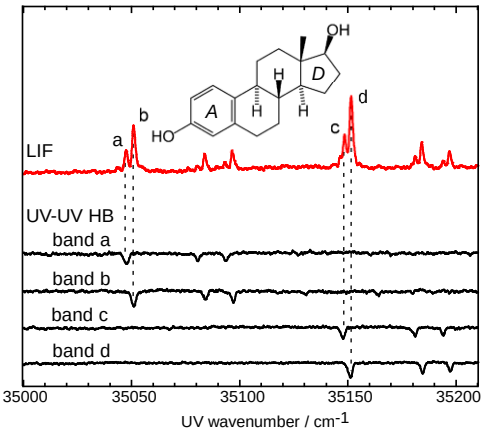
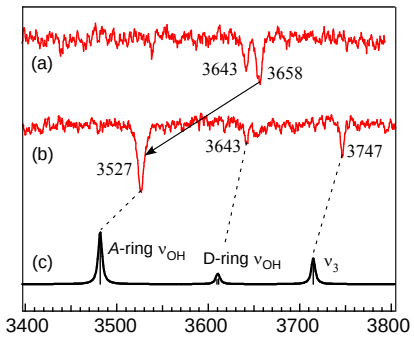
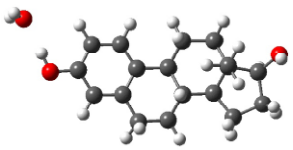


Fig. 1 LIF spectrum and UV-UV HB spectra of bare E_2.

Experiment: Jet-cooled E_2 and its hydrated clusters are generated by an adiabatic expansion of gaseous mixture of sample and He carrier gas (and water vapor) in a vacuum chamber. Electronic spectra were measured by laser induced fluorescence(LIF). For distinguishing vibronic bands due to different species in the jet, UV-UV hole burning(HB) spectroscopy were applied. Infrared spectra were measured by IR-UV double resonance(DR) spectroscopy.

Result and discussion: Fig. 1 shows S_1-S_0 LIF and UV-UV HB spectra of E_2. In 35040-35200 cm^{-1} region, there are four prominent bands (a)-(d). We concluded that they due to four conformers for bare E_2 arising from the orientation of the phenolic OH(A-ring OH) and the OH in the five-membered ring(D-ring OH). Fig. 2 shows IR-UV DR spectra of one of (a) bare E_2, (b) 1:1 hydrated cluster. In spectrum (a), two OH stretching bands are observed. In spectrum (b), the band at 3658 cm^{-1} of bare E_2 is shifted to 3527 cm^{-1}. In addition, ν_3 of H_2O is observed at 3747 cm^{-1}. Fig. 2 (c) shows calculated IR spectrum for stable structure of 1:1 hydrated cluster forming the H-bond on A-ring OH obtained at M05-2X/6-311++G** level. The calculated spectrum reproduces the observed IR spectra. We will discuss other conformers of bare E_2 and 1:1 hydrated clusters.





Estradiol-(H_2O)

Fig .2 IR-UV DR spectra of (a) bare E_2, (b) E_2-(H_2O) and calculated IR spectra of (c) E_2-(H_2O) exhibiting in lower panel.