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Ultrafast N–H vibrational dynamics of hydrogen-bonded cyclic amide reveal by 2DIR spectroscopy

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This article is dedicated to Prof. Wolfgang Domcke on the occasion of his 70th birthday

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ABSTRACT

Hydrogen-bonding strongly influences the vibrational dynamics of the N–H stretch vibration, hence the molecular structure and dynamics. Therefore the N–H stretch vibration is an important probe to study hydrogen-bond dynamics as well as the molecular structure and dynamics, specially for the biological molecule. In this article, the dynamics and couplings of N–H stretching vibrations of biological molecules are investigated with linear infrared spectroscopy and ultrafast two-dimensional infrared (2DIR) spectroscopy with a model molecule 2-Pyrrolidinone. In solution, 2-Pyrrolidinone makes three different kinds of intermolecular hydrogen bonding, whose spectra have been collected with FTIR as well as with 2DIR spectroscopy and discussed. Inter-molecular hydrogen bond making and breaking between N–H and C=O vibrational bands are discussed also.

1. Introduction

Hydrogen-bond plays an essential role on biological activities [1–4]. For example, hydrogen-bonding stabilizes protein structure, therefore control the biological processes, like protein folding, substrate binding, molecular recognition, self-assembly, etc [5–8]. The specific hydrogen-bonding configuration and strength have a large impact on the biological structure and dynamics [9–11]. Modulations of the hydrogen-bonding environment, e.g., the hydrogen-bond stretch and twist modes, effects the vibrational dynamics of the molecules [12–14]. Therefore, a detail understanding of hydrogen-bond characteristics of the biological molecules is an essential task to understand the biological activities. Although the hydrogen-bond is a text book study, however its mechanism is still not understood well, due to the extreme fast evolution of the hydrogen-bond networks [15,16]. The development of new technologies, specially the development of ultrafast multidimensional spectroscopy [17–19], facilitate a detail understanding of the molecular structure and dynamics along with the inter- and intra- molecular interaction, down to femtosecond time resolution [20,21]. In particular two dimensional infrared spectroscopy (2DIR) seems to have a high potential to reveal the hydrogen-bond dynamics in detail [22–24].

In 2DIR spectra, the structural information is encoded in the strength, position, and shape of off-diagonal cross-peaks which are not directly observable in one-dimensional absorption spectra [25–28]. Additionally, the 2DIR snapshots, taken at different population times, provide structural and dynamical information of the molecule [29]. In principle it is possible to observe hydrogen bond dynamics by taking a sequence of 2DIR snapshots [30,23]. However the direct observation of hydrogen-bond dynamics still is a challenge. On the other hand, since hydrogen-bonding changes the force constant of the participating functional groups, as a consequence their vibrational frequency also change [31,32]. Therefore, it is possible to realise hydrogen-bond characteristics by observing the vibrational dynamics of the participating functional group. In biological molecule, amide-I, which is essentially the C=O stretch vibration at around 1700 cm^{-1} and amide-A, the N–H stretch vibration at around 3400 cm^{-1}, both make hydrogen-bonding with one another (N–H···C=O) as well as with water molecules, leading to shifts the respective vibrational frequencies. The shift of the vibrational frequency of amide-I and amide-A depends on the strength and number of hydrogen-bonds formed with the functional group. For example, a red shift of the amide-I frequency by approximately 16 cm^{-1} is observed when a single hydrogen-bond is formed between the amide-I oxygen atom and a water molecule [33]. In case of amide-A band, the frequency shift can be up to few hundreds of wave number. Therefore hydrogen-bonding can be probed by monitoring the frequency shift of the amide-I or amide-A band, which decreases with increased strength of the hydrogen-bonding [23,34]. Compared to the amide-I band, the amide-A undergoes a large frequency shift due to the hydrogen-bonding. Therefore, it is easier to understand the hydrogen-bonding by probing the amide-A band.

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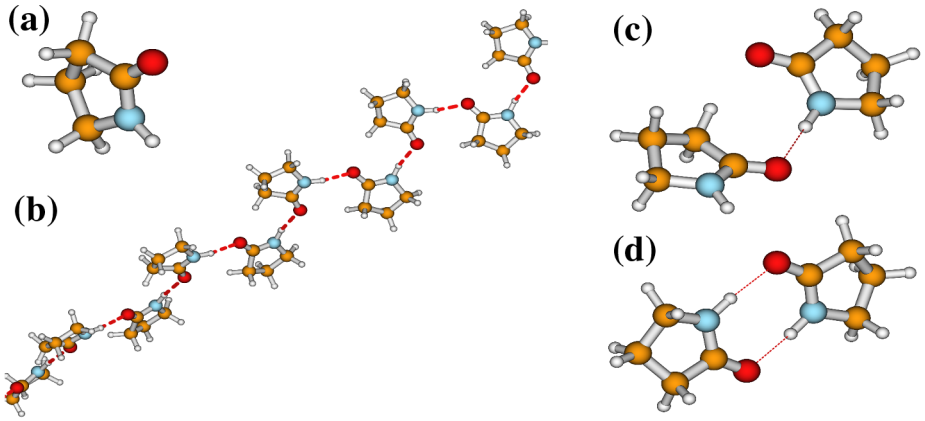

Fig. 1. Molecular structure of 2-Pyrrolidinone and its hydrogen bonded oligomers. The red dashed line between molecules indicates the intermolecular hydrogen bond. (a) 2-Pyrrolidinone monomer, (b) single hydrogen bonded oligomer (SHBO), (c) single hydrogen bonded dimer (SHBD), and (d) doubly hydrogen bonded dimer (DHBD).

In general, the hydrogen-bonded molecules in solution often give rise to broad, not seldom featureless vibrational spectra due to the inhomogeneous broadening, which makes it difficult or impossible to uncover the underlying dynamics. A simple small molecule is then necessary for a detail understanding of the hydrogen-bond characteristics. The cyclic amide 2-Pyrrolidinone can form the hydrogen-bonds similar to the peptides and therefore can be used as a simple model system to study the dynamics of the hydrogen-bonded molecular systems [35]. Moreover, in solution, 2-Pyrrolidinone molecules form three different kinds of inter-molecular hydrogen-bonding, e.g. single hydrogen-bonded dimer (SHBD), doubly hydrogen-bonded dimer (DHBD) and single hydrogen-bonded oligomers (SHBO), which allow to study a variety of structural features relating to the hydrogen-bonding. The different hydrogen-bonding structures of 2-Pyrrolidinone are depicted in Fig. 1.

2. Experimental procedures

An Ultrafast regenerative/multi-pass Ti:Sapphire amplifier (Integra-C, Quantronix) is used to obtain initial femtosecond pulses at 800 nm. The output of the amplifier consist of 100 fs transform-limited 2.5 mJ pulses at a 1 kHz repetition rate. This output beam is split into two (60: 40) which pump two OPAs (TOPAS, Light conversion). With the non-collinear difference frequency generator (NDFG, Light conversion) both OPAs are optimized to generate infrared pulses centered at 3250 cm^{-1}. The highest power output pulse is chosen as the pump beam and the other pulse serves as probe in 2DIR measurements.

To perform the two dimensional photon echo experiment in pump-probe geometry, the pump beam is split into two beams to produce two pump pulses. Both pump pulses are reflected back from two retro-reflectors placed on two independently computer controlled translation stages which create the time delays between different pulses. Finally both the pump pulses are overlapped by using a zinc selenide (ZnSe) beam splitter, so that they can propagate collinearly and then focus on the sample at the same point by an off axis parabolic mirror. The probe pulse is also focussed on the sample using the same off axis parabolic mirror and crosses the pump pulses inside the sample with a small angle (about 12°). Details of the experimental setup are described elsewhere [36].

To produce and detect the echo signal, one of the pump pulses is chopped by an optical chopper with a frequency of 500 Hz. The vibrational echo signal is created inside the sample due to the interactions of three excitation pulses and emitted in the same direction as the probe beam. The probe beam itself acts as a local oscillator (LO) and perform self-heterodyne-detection of the echo signal. The echo signal is detected by spectral interferometry which directly gives the echo as a function of the detected frequency ω_m. The coherence time τ is then scanned at constant population time T_w and the signal is Fourier-transformed along the τ dimension to produce the excitation frequency dimension ω_τ. The signal is spectrally resolved using the Horiba Jobin Yvon iHR320 spectrometer and is detected by a 64 elements MCT double array (from Infrared Systems Development).

The sample (2-Pyrrolidinone C_4H_7NO) is purchased from Sigma-Aldrich with 99.9% purity and dissolved in carbon tetrachloride (CCl_4 with 99.9% purity) without any further purification. The concentration of the sample is optimized to 20% by volume to perform the experiment with a reasonable signal strength. A home made, specially tailored sample cell consisting of two 2 mm thick CaF_2 windows, separated by a 15μ Teflon spacer, is used to hold the sample for photon echo measurements. All the experiments have been performed at room temperature (21 °C). The whole system is purged with dry air to remove the water vapor from the system.

3. Results and discussions

The experimental one-dimensional FTIR absorption spectra of 2-Pyrrolidinone in carbon tetrachloride (20% by volume concentration) measured in amide A stretch vibrational region (3000–3550 cm^{-1}), is presented in Fig. 2. Essentially amide A band is the N–H stretch vibration of 2-Pyrrolidinone, it is expected to be present at around 3450 cm^{-1} spectral position [37]. Indeed a narrow very low intense peak is observed at around 3450 cm^{-1}. However, a strong absorption peak is observed around 3212 cm^{-1} along with few shoulder peaks. The origin of this peak and it's shoulder peaks are explained in the following sections.

A very broad band (FWHM ca. 165 cm^{-1}), strong absorption peak is observed at around 3212 cm^{-1}. This broad peak is identified as the N–H stretch vibrational frequencies from SHBO. In room temperature, a large distribution of molecular chains of SHBO present in the sample. The vibrational frequency of the N–H bond of SHBO highly depend on the number molecules present in the chain. The hydrogen bond strength increases in SHBO as the chain length increases. As a result, a broad

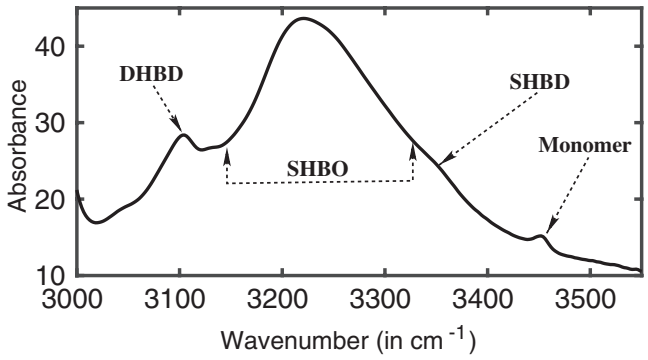

Fig. 2. The linear FTIR absorption spectra in the N–H stretch vibrational region of 2-Pyrrolidinone in carbon tetrachloride.

spectral distribution is observed where N–H vibrational frequency is red shifted with the increase chain length of SHBO. This broad peak is highly asymmetric and the slope of the spectral envelop reflects the distribution of chain length of oligomers. It is clear from the slope that the population distribution of oligomers slowly increase (right side of the peak) to an optimal chain length, where as the population of longer chains drop very quickly (left side of the peak) after reaching the optimal chain length. In spite of the asymmetry of the peak, both the ascending and descending slopes are very smooth, which indicates a systematic change of the population of the oligomers chain length. In contrast, SHBD is identified with a very small hump at around 3360 cm^{-1} (see Fig. 2). The population of SHBD is higher than expected due to the intermediate state of hydrogen bond breaking and making processes among DHBD and SHBO molecular chain. A detail explanation is in section below.

A prominent absorption peak is observed at around 3106 cm^{-1} and is identified as N–H stretch vibrational frequency of DHBD. The stronger absorption peak of DHBD than SHBD (see Fig. 2) indicates that, the population of DHBD is higher than the SHBD. The reason for the higher population of DHBD is its higher stability due to the stronger hydrogen bonding. In DHBD, the hydrogen-bond donor and acceptor from two molecules make hydrogen-bonding with each other, hence possess stronger binding with each other. Therefore once DHBD is formed, remain in this stable configuration for longer time period. On the other hand, due to the presence of the free hydrogen-bond acceptor and donor terminal in SHBD, both the terminals try to make hydrogen-bonding with other molecules and form a molecular chain or make bonding itself and form a DHBD. The molecular chain formation is depicted in Fig. 3. As a result, population of DHBD in solution is higher than SHBD and yield a stronger absorption peak at 3106 cm^{-1}. Other than the pure 2-Pyrrolidinone, there are always few monomers present in the solution and appear as a weak narrow peak at around 3452 cm^{-1}.

In contrast to linear absorption spectra, two dimensional infrared spectra provide further information about the dynamical character of the ultrafast N–H vibration and hydrogen-bond dynamics. Two dimensional echo spectra of the N–H stretch vibrational region of 2-Pyrrolidinone at a population time T_w = 600 fs is presented in Fig. 4. The excitation frequency is plotted on the horizontal axis, whereas the detection frequency is on the vertical axis. For a better understanding of the peak position, the linear absorption spectrum is embedded on the top and the right side of the 2DIR spectra. The dotted arrows from the linear spectra to the 2DIR spectra give a better understanding of the

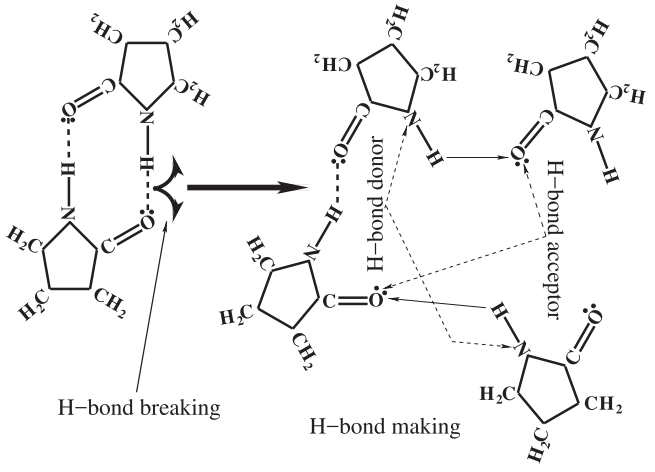

Fig. 3. The hydrogen-bond breaking and making processes. In the left side, one of the hydrogen-bond from a DHBD breaks and forms a SHBD. In the right side, this SHBD, makes hydrogen bonding with another two monomers and forms a molecular chain, the SHBO.

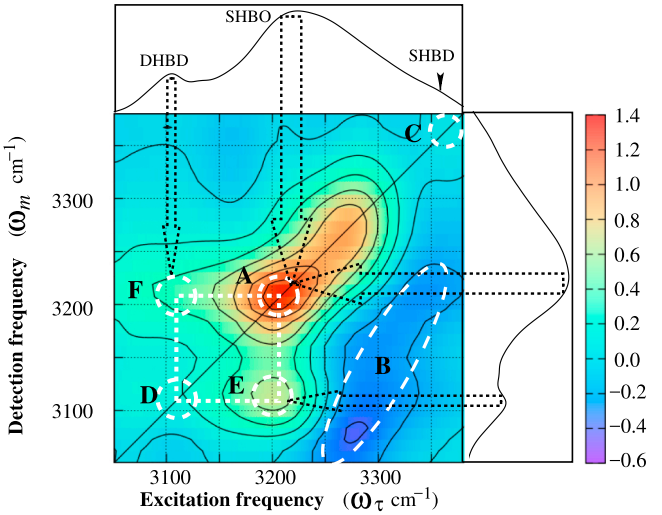

Fig. 4. Two dimensional vibrational photon echo real spectra of 2-Pyrrolidinone at the N–H stretch vibrational region in carbon tetrachloride at a population time T_w = 600 fs. The red contours are the positive trending and the blue contours are the negative trending. The horizontal axis is the Fourier transformed τ-axis (ω_τ) and the vertical axis is the monochromator axis (ω_m). The embedded one dimensional spectra is the FTIR absorption spectra. Both the linear and two dimensional spectra are acquired at room temperature.

peak positions. The colour spectrum on the right side, scales the 2DIR spectral strength.

A very broad and strong positive peak (**A**) is observed on the diagonal at around 3225 cm^{-1} (see Fig. 4). The peak intensity is not uniform, rather asymmetrically distributed along the diagonal. The asymmetric intensity distribution of the peak, exactly follows the linear absorption spectral intensity pattern, which is identified as the hydrogen-bonded N–H stretch vibrations for SHBO. Therefore, this positive diagonal peak is caused by the ground state bleaching and excited state emission of the hydrogen-bonded N–H stretch vibrational band of SHBO. A negative peak (blue peak, "**B**") is observed in parallel with the diagonal N–H stretch vibrational peak. This negative peak is due to the excited state absorption of the hydrogen-bonded N–H vibrational band. A deformation of this negative peak is observed due to the overlap of a positive cross peak (3200 cm^{-1}, 3106 cm^{-1}), which arises at the lower frequency side of the negative peak. Origin of this positive peak is explained in next section.

A diagonal peak is expected at around ($\omega_\tau = \omega_m$=3360 cm^{-1}) due to the N–H stretch vibration of SHBD. However, the peak intensity is expected to be very low, according to the linear absorption spectra (see Fig. 2). Nevertheless, a very low intensity diagonal peak (**C**) is observed at the top right corner of the 2DIR spectra. This peak is due to the ground state bleaching and excited state emission of the hydrogen-bonded N–H stretch band of SHBD. A diagonal peak from monomer should appear at around ($\omega_\tau = \omega_m$=3452 cm^{-1}), however, the laser spectrum used for the experiment is not broad enough to observe the monomer peak along with hydrogen bonded N–H peak, therefore it is not observed in 2DIR spectra in Fig. 4.

A weak peak is expected to be present on the diagonal at ($\omega_\tau = \omega_m$=3106 cm^{-1}) due to the N–H stretch vibration of DHBD. However, due to the surrounding high intense peaks, it is not clearly visible. The position of the peak is marked with a white circle **D**. Nevertheless, the existence of this diagonal peak is indicated by two off-diagonal positive peaks at around (ω_τ=3210 cm^{-1}, ω_m=3106 cm^{-1}, "**E**") and (ω_τ=3106 cm^{-1}, ω_m=3210 cm^{-1}, "**F**"). These two off-diagonal peaks form a square pattern along with the diagonal peaks at **A** and **D**. This square feature points to the hydrogen-bond breaking and making mechanism of DHBD and SHBO. In one process, one of the hydrogen-bonds from a DHBD breaks and makes another hydrogen-bond with a

long chain and leads to the off-diagonal peak **F**. In another process, the second last hydrogen bond in a long chain breaks, thus forming a SHBD. The open acceptor and donor terminal of SHBD come closer and make hydrogen bonding and finally DHBD is formed. This process leads to a positive off-diagonal peak **E**. The breaking and making of hydrogen-bonding is depicted schematically in Fig. 3. According to the off-diagonal peak position, it is clear that the chains longer than the optimal chain length are more likely to take part in hydrogen-bond breaking and making processes. This hydrogen-bond making and breaking processes are bi-directional and stabilized with the temperature. However, due to the hydrogen-bond breaking and making among DHBD and long chain oligomers, there are always few intermediate SHBDs, as a result, there are on average more SHBD than it expected, which yields a noticeable absorption peak at around 3360 cm^{-1} on the linear absorption spectra (see Fig. 2).

4. Conclusions

The ultrafast N–H stretch vibration of the hydrogen-bonded 2-Pyrrolidinone has been studied with linear absorption spectroscopy as well as with ultrafast 2D-IR spectroscopy. The combination of both spectra provide a quantitative understanding of the hydrogen-bonded N–H stretch vibration. A large distribution of molecular chains are formed due to the hydrogen bonding which yield a broad spectra with FWHM of 165 cm^{-1}. The N–H stretch vibration is red shifted as the chain size of SHBO increase. The distribution of molecular chain length is not uniform with respect to the optimal chain length, rather a slow increase of population of the chain length is observed up to optimal chain length, and a very fast drop of population is observed for the molecular chain longer than the optimal chain length. The strongest hydrogen bonding is observed for the doubly hydrogen bonded dimer, which shows a strong red shift of the N–H vibrational band. The cross peaks near the red side of the N–H diagonal peak, confirm the hydrogen bond making and breaking dynamics between DHBD and SHBO.

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