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Conformational stability of DNA in hydrated ionic liquid by synchrotron-based UV Resonance Raman

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ABSTRACT

Although Deoxyribonucleic acid (DNA) is considered substantially stable in aqueous solution, slow hydrolysis can damage its double-helix structure and cause denaturation when it is stored for several months. Therefore, the design of aqueous solvents that are able to stabilize and maintain DNA conformation is a challenging issue. Ionic liquids (ILs) appear as ideal water co-solvents for DNA biotechnology due to their unique properties. We have investigated the thermal stability of DNA in 1-butyl-3-methylimidazolium aqueous solutions by synchrotron-based UV Resonance Raman (UVRR) spectroscopy with the aim to clarify the role played by concentration of IL in stabilizing the DNA natural conformation. The synchrotron-based UV source for UVRR measurements allows us to enhance specific vibrational signals associated to nitrogenous bases of DNA, through an appropriate tuning of the excitation wavelength. Such approach permits to probe the rearrangements in the local environment around specific nucleotides as a function of thermal conditions.

Keywords: UV Resonance Raman scattering, DNA, ionic liquid, melting transition

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1. INTRODUCTION

Deoxyribonucleic acid (DNA) is a macromolecule of pivotal biological role thanks to its ability to store the genetic instructions for the growth, functioning and development in the cell. It plays key role in many biological processes, i.e. gene expression transcription and carcinogenesis[1]. Due to its properties together with its chiral structure[2], DNA represents a key component in pharmaceutical and biomedical studies and a crucial material in the development of advanced molecular device[3,4]. From a structural point of view, DNA is composed of two linear stands of nucleotides that coil around each other to form the characteristic double helix structure. Each nucleotide is composed by a phosphate group, a deoxyribose monosaccharidic unit and one of the four nucleobases (cytosine, guanine, adenine and thymine). The nucleobases of the two chains interact by H-bond, according to the base-pairing rules, connecting the two sugar-phosphate backbones. Figure 1 reports a representative chemical structures of DNA for two Watson-Crick base-pairs with the conventions adopted for the numbering of atoms. Although DNA is considered stable in aqueous solution, slow hydrolytic reactions such as deamination and depurination may denature the double helical DNA conformation[5] For this reason, a growing interest has been devoted to the development of suitable aqueous solvents able to improve the stabilization of DNA[6,7]. This could open the possibility to maintain the native DNA structure for a long period and in critical conditions, such as high temperature and pressure[8].

Ionic liquids (ILs) have proven to be the preferred solvents to replace the traditional organic solvents and/or aqueous solution in many types of reactions[9, 10]. They are composed by anions and organic cations whose structure is such to make the lattice enthalpy low, thus resulting in low melting points. They are characterized by interesting properties such as negligible vapor pressure, non-flammability, high thermal and chemical stability and low toxicity[11, 12]. Based on these peculiarities, ILs find applications in organic synthesis[13], electrochemical devices[14], photochemical cells[15, 16] and catalysis[17]. During the last years, the application of ILs to DNA technology has received particularly attention. For instance, in literature it is reported the use of ILs for the extraction of trace amount of DNA from the aqueous solution[10], for slowing DNA translocation through nanopores[18] and for the DNA storage[19]. All such applications are strongly dependent on the interaction at molecular level between ILs and DNA. A basic understanding of IL-DNA

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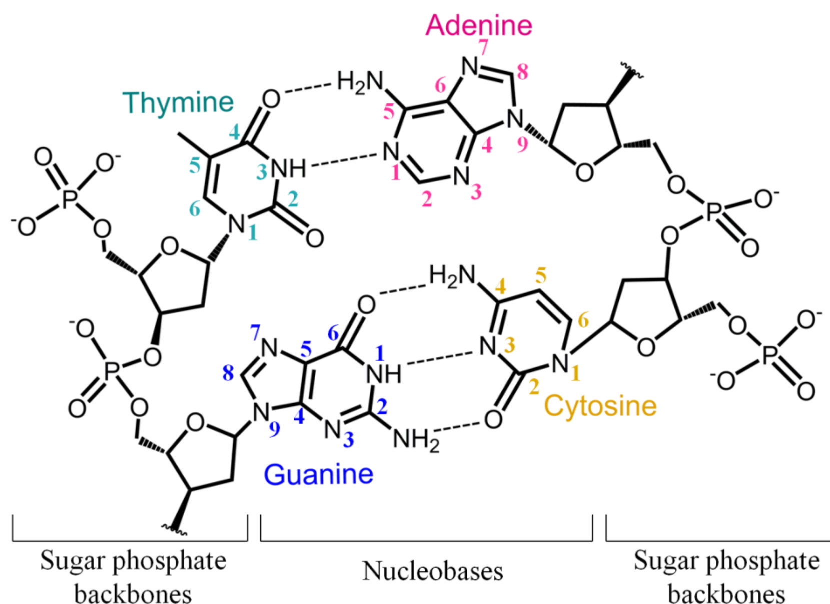

Figure 1: Chemical structure of DNA for adenine-thymine and guanine-cytosine base pairs. Dashed lines represent Watson-Crick H-bonds.

interaction could drive to a tailored use of ILs in various fields of life science. Several theoretical studies investigate the interaction of DNA with pure ILs and/or with IL/water solutions. Molecular dynamics simulation results suggest that both the groove binding mechanism of IL cations and their electrostatic association with DNA backbone contribute significantly to DNA stability[20, 21]. However, no experimental findings are present in the literature in support of this hypothesis. DNA/IL systems are widely investigated by circular dichroism, fluorescence and UV/Vis spectroscopies[19, 22-24]. However, these techniques provide information on the stabilizing or destabilizing effect of ILs on the DNA natural conformation, but do not provide detailed information on the molecular interactions causing such effects. A comprehensive experimental picture in terms of molecular interactions involved in DNA/ILs and the thermodynamics of the interaction process is still missing.

In the present work, we explore the thermal stability of DNA in water in presence of an increasing concentration of imidazolium-based chloride by synchrotron-based UV Resonance Raman (UVRR) scattering[25]. This technique represents a powerful tool for investigating the nature of inter-molecular interactions established between the IL cations and DNA bases. This is due to the selectively enhancement, in resonance conditions, of the vibrations mainly localized on nucleotides ring. This allows to minimize the Raman signals associated with the phosphate and sugar backbones, as well as those arising from buffer and solvent[26-27], thus simplifying the complex Raman spectra of DNA. Moreover, the tunability of UV synchrotron radiation source permits a careful choice of the excitation wavelength in correspondence of the electronic transitions of specific nucleobases. Such approach allows to disentangle in a very efficient way the contributions arising from individual bases in the spectra of DNA[28]. In particular, the choice of 250 nm as excitation wavelength gives the opportunity to enhance and isolate the ring in-plane vibration associated to the guanine residues[29]. This Raman feature is highly sensitive to the thermal disordering and it can be used as molecular marker of thermal denaturation of DNA.

2. MATERIALS AND METHODS

2.1 Samples preparation

1-Butyl-3-methylimidazolium chloride ([C_4MIM]Cl) was purchased by IoLiTec with a purity of 99%. Before the use, IL was previously dried under vacuum with phosphorus pentoxide for 48hs in order to remove any water contamination.

DNA sodium salt from salmon testes (2000 base-pairs, CAS number 438545-06-3) was purchased by Sigma-Aldrich and used without further purification. The absence of proteins as contaminants[30] was checked by measuring the absorbance ratio of a DNA solution at 260 and 280 nm that was found to be equal to 1.9. Trizma and Trizma-HCl were purchased by Sigma-Aldrich. For the preparation of solutions to be measured, a DNA stock solution of

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1mg/mL was prepared by dissolving dry DNA in Tris 10mM at pH 7.4 and gently stirring for 24 h up to reaching a limpid solution. A detailed description of DNA/IL samples preparation is reported in Table 1:

Table 1: Description of DNA/IL samples preparation.

	DNA in Tris	DNA in $[C_4MIM]Cl$		
DNA/IL	1/0 (w/w)	1/22 (w/w)	1/44 (w/w)	1/87 (w/w)
Preparation	250 µL of DNA stock sol. 750 µL of Tris	250 µL of DNA stock sol. 745µL of Tris 5µL of $[C_4MIM]Cl$	250µL of DNA stock sol. 740µL of Tris 10 µL of $[C_4MIM]Cl$	250 µL of DNA stock sol. 730 µL of Tris 20 µL of $[C_4MIM]Cl$

2.2 UVRR scattering

UVRR experiments were carried out at the BL10.2-IUVS beamline of Elettra Sincrotrone Trieste (Italy)[25]. UVRR spectra were excited at 250 nm by exploiting the UV emission provided by the synchrotron radiation (SR) source Elettra. UVRR spectra were recorded in back-scattered geometry by using a Czerny-Turner spectrometer (Trivista 557, Princeton Instruments) with a spectral resolution of ≈ 15 cm^{-1}. The radiation power on the sample was ~20 µW. Any possible photo-damage effect due to a prolonged exposure of the sample to UV radiation was avoided by continuously spinning the sample cell during the measurements. For each sample, UVRR spectra were recorded in the temperature range from 305 to 370 K. In order to compare the DNA spectra in presence and absence of ILs at a given temperature, the experimental profiles were normalized via the intensity of the OH stretching band of water at ≈3400 cm^{-1} [29,31].

3. RESULTS AND DISCUSSION

Figure 2 shows the temperature-evolution of UVRR spectra excited at 250 nm and collected for DNA/IL = 1/22 (w/w). In the wavenumber region between 1300 to 1800 cm^{-1}, it is noteworthy the behaviour of the band centered at ~1487 cm^{-1} and labeled as band I. This peak is mainly attributable to guanine residues[29] arising from a combination of bending motion of C8-H and stretching movements of C8=N7 and N9-C8 (see Figure 1)[27,31]. Figure 2 shows an

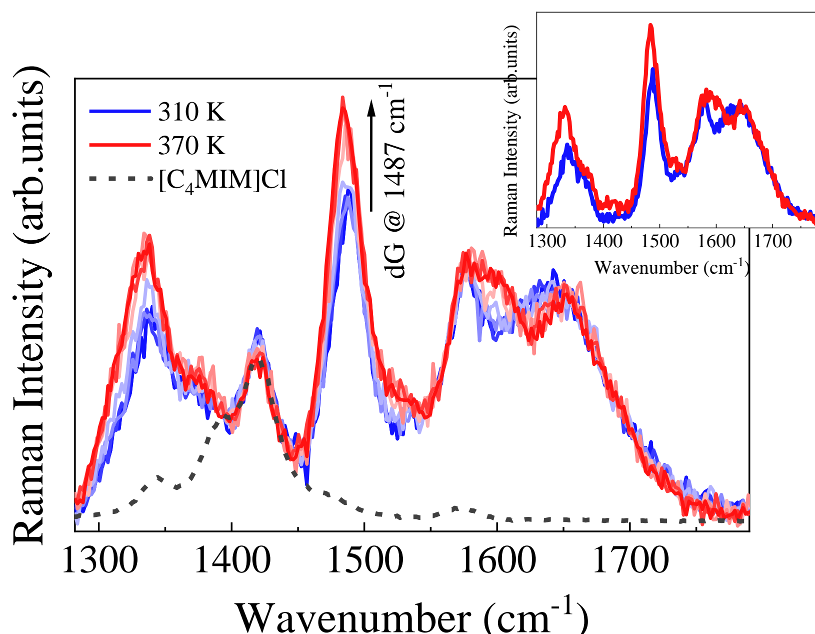

Figure 2: Temperature-evolution of UVRR spectra of DNA/IL (1/22 w/w). The dashed-lines represent the UVRR spectra of pure $[C_4MIM]Cl$. Inset: Comparison between the UVRR spectra of DNA/IL (1/0 w/w) collected at 305 and 370 K.

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increment of the intensity of the band I as a function of temperature both for DNA/IL = 1/22 (w/w) and for pristine DNA (see Inset of Figure 2). This trend, i.e. Raman hyperchromic effect[32] recalls to the UV absorbance hyperchromism observed for DNA and it reflects the interdependence between the Raman scattering cross-section and the electronic absorption intensity. Consistently with UV absorbance, the increment of the Raman intensity of the aromatic ring vibrations of nucleotides is related to the thermal denaturation of DNA promoted by the increasing of temperature. This process has been ascribed, at molecular level, to two different effects: i) the disruption of vertical base-base stacking interactions and ii) the breakage of hydrogen bonds (HB) between Watson-Crick base pairs of DNA[33-35].

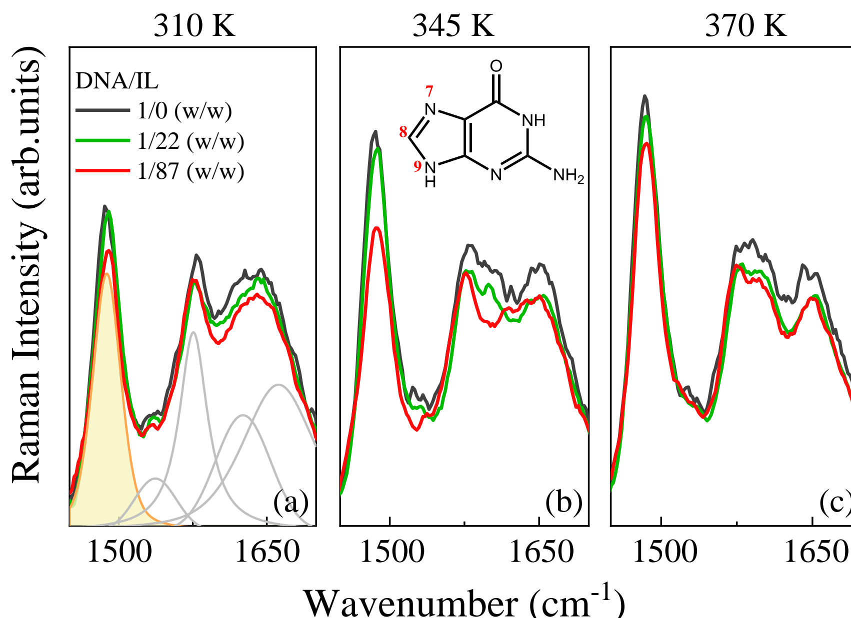

Figure 3: Comparison between the 250 nm-excited Raman spectra of DNA/IL as function of concentration of [C_4MIM]Cl at T=310 K (a), 345 K (b) and 370 K (c) in the wavenumber range 1450-1700 cm^{-1}. Representative fitting procedure is reported.

Figure 3 displays the variation in intensity undergone by band I as a function of the increasing concentration of [C_4MIM]Cl at three representative temperature. In order to better compare the spectra, the vibrational contribution of IL was subtracted from the total spectra of DNA+IL, after appropriate normalization on the intensity of the Raman signals assigned to the vibrational modes of [C_4MIM]Cl at 1021, 1095 and 1213 cm^{-1}. The reliability of this procedure is ensured by the fact that in the spectra region between 1000 and 1200 cm^{-1} Raman features arising from DNA are practically negligible with respect to the signals of IL. In order to extract more quantitative parameters that account the effect of IL concentration on the intensity of band I, a decomposition procedure of the spectra has been performed. An example of best- fitting procedure for the spectrum of DNA/IL = 1/87 (w/w) collected at 310 K is reported in Figure 3 for the wavenumber range of interest.

Figure 4 shows the temperature-dependence of the UVRR intensity of the band I for pristine DNA and at different percentages of [C_4MIM]Cl. As common feature to all the trends, it can be observed a sharp upturn for the intensity of the band I in correspondence of ≈340-350 K. This temperature range is usually associated to the melting transition of DNA that involves the full denaturation of the double-stranded structure[34,36]. By inspection of Fig. 4, it is possible to observe that the intensities of band I for the spectra of DNA in presence of IL are less intense with respect to those measured in pure DNA over the whole investigated temperature range. This hypochromic effect suggests that the addition of [C_4MIM]Cl tends to favor the formation of a more compact structure in DNA double-stranded[29]. Moreover, the persistence of hypochromicity also after the unfolding of DNA gives indication that the base-stacking of guanines is quite effective for DNA in the presence of [C_4MIM]Cl. The plots in Figure 4 point out also a slight increment of the melting temperature observed for DNA as a consequence of the progressive addition of IL. In order to extract quantitative information, the intensity $I(T)$ of the band I can be properly described by a two state model[37] following the eqn:

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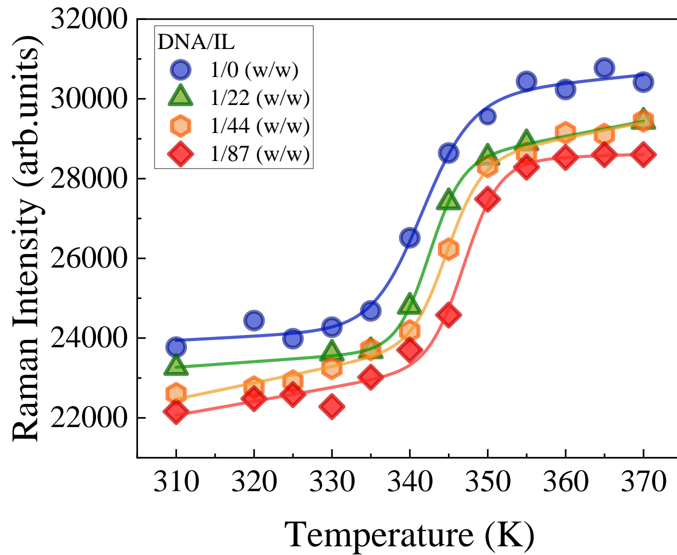

Figure 4: Temperature-dependence of the Raman intensity of the band I for DNA/IL (w/w) = 1/0 (blue circles), 1/22 (green triangles), 1/44 (orange hexagons), 1/87 (red rhombs). Continuous lines are fitting of the experimental data by using eqn. (1), see details in the text.

$$I(T) = \frac{I_N + m_N \cdot T + (I_D + m_D \cdot T) K_T}{1 + K_T}, \quad (1)$$

where K_T signifies the equilibrium constant between native and denaturated states, I_N and I_D represent the intensities corresponding to the native and denaturated state of DNA, respectively. In the equation above, the parameters m_N and m_D describe the linear temperature-dependence of the band intensity in the pre and post-melting regions, respectively. Finally, the equilibrium constant native and denaturated states can be expressed as:

$$K_T = \exp\left[\frac{\Delta H_m}{R}\left(\frac{1}{T_m} - \frac{1}{T}\right)\right], \quad (2)$$

where R is the gas constant and ΔH_m and T_m are the enthalpy variation and the temperature associated to the melting process.

As visible in Figure 4, the temperature-dependence of the band I is satisfactorily reproduced by using eqn (1). The fitting procedure of plots in Figure 4 provides the estimation of the parameters ΔH_m and T_m, as summarized in Table 2.

Table 2: Thermodynamic parameters extracted by fitting the experimental data of Fig 4 with eqn (1) (see text for details).

DNA/IL	T_m (K)	ΔH_m (kJ/mol)
1/0 w/w	341.6 ± 0.5	3025.1 ± 736.4
1/22 w/w	342.5 ± 0.5	4640.1 ± 288.7
1/44 w/w	344.8 ± 0.5	4380.6 ± 849.3
1/87 w/w	347.3 ± 0.5	5096.2± 673.6

The values reported in Table I confirm the slight increment of the melting temperature induced by the increasing concentration of [C_4MIM]Cl, as already discussed above. This may be consistent with the results of theoretical investigations[20,21] suggesting that the cations of IL tend to majorly interact with the DNA backbone when the negative charges of phosphate groups are localized. This implies that the cations are able to stabilize the DNA structure by reducing charge repulsion between the phosphate groups on each of the DNA strands[38]. This stabilization effect is probably accompanied by the establishment of so-called H-bond interactions between the CH groups of IL[20] and the acceptor/donor sites present on the major and minor grooves of DNA. Overall these effects result in an enhancement of the stability of DNA native conformation also at higher temperature, promoted by the

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presence of IL. The presence of IL induces an increase of ΔH_m value with respect to the case of DNA/IL = 1/0 (w/w). This result is in analogue with other investigation on melting parameter of DNA with divalent metal cations[38].

Beside the intensity change, Figure 4 points out also a slight red-shift for the band I upon the increasing of thermal motion. Figure 5 reports the wavenumber positions of band I found for pristine DNA and DNA+IL. Due to the normal composition of band I, the frequency of this Raman peak is sensitive to the interactions between the solvent molecules and the N7 site of guanine that can act as acceptor of H-bond[39-40]. The shift of the band I to lower frequency with the thermal denaturation has been attributed to a reinforcement of H-bond formed by guanine with the solvent[33]. This phenomenon can be can be attributed to a major exposure of N7 site in denaturated DNA to solvent molecules. By the inspection of figure 5, we note that before the DNA thermal denaturation the presence of IL induces a slight blue-shift in the position of band I with respect to the case of pristine DNA. This result can be likewise explained by considering two effects: i) the formation of so-called H-bond interaction on N7 atom with CH groups of [C_4MIM]Cl[20] and ii) the reduction of H-bond interaction between buffer solvent molecules and N7 site due to the presence of cations of IL[41]. Since it is well-known the capacity of cations of IL to penetrate the “cone of hydration” of water molecules around the charged phosphate groups of DNA[21], the diffusion of water across the nucleobases in DNA is hampered by the presence of IL. This is consistent with the slight blue-shift of band I observed in the samples of DNA+IL with respect to pure DNA before the melting temperature. The disappearing of this effect at high temperatures (see Figure 5) is probably due to the alteration of DNA structure caused by the melting process.

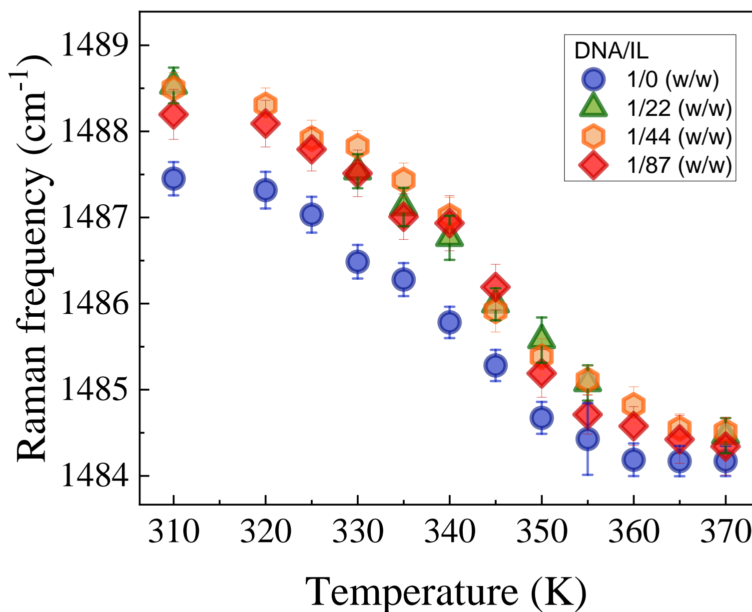

Figure 5: Temperature dependence of wavenumber position for the band I for pristine DNA and DNA+IL DNA/IL (w/w) = 1/0 (blue circles), 1/22 (green triangles), 1/44 (orange hexagons), 1/87 (red rhombs).

4. CONCLUSIONS

We presented the results of synchrotron-based UVRR investigation on the temperature-dependent structural stability of DNA in presence of [C_4MIM]Cl as function of DNA/IL ratio. The choice of 250 nm as excitation wavelength gives the possibility to selectively enhance the vibrational signals associated to aromatic ring of guanine residues, then simplifying the complex off-resonance Raman spectra of DNA. The experimental data suggest that the thermal stability of DNA in IL is related at molecular level by two mechanisms: i) the unstacking of guanine bases and ii) the intermolecular interactions involving the N7 site of guanine. As main result, the thermal stability of DNA is found to increase as function of concentration of [C_4MIM]Cl in the investigated DNA/IL ratio range.

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