UV Raman and Brillouin scattering experiments for probing solute-solvent interactions in cyclodextrin aqueous solutions

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The investigation of structural and dynamical properties of aqueous solutions of sugars is a fundamental topic for the deep comprehension of important biological mechanisms of animals and plant life. Due to the very broad time/length scale which characterizes the molecular restructuring processes taking place in aqueous solutions, a wide range of different experimental techniques has been developed during the years in order to achieve a comprehensive view of the mechanisms that drive the solvation dynamics of biomolecules. In this contribution, we will show how the joint use of UV inelastic scattering experiments, i.e. UV Raman and Brillouin spectroscopy, can be implemented for probing in a complementary way the solute-solvent interactions and the hydration shell behaviour in aqueous solutions of cyclodextrins (CD). CD are oligosaccharides composed of a variable number of glucose units that exhibit remarkable properties of molecular host systems. Thanks to this ability together with their biocompatibility, CD have found in these years many industrial uses, including in the food, cosmetic and pharmaceutical field. Water plays an important role in determining the performances of CD and their derivatives as host molecules. The continuous breaking/reformation of hydrogen-bonds (HB) between the solute and the solvent and the dynamic re-organization of water molecules at the interface of the CD can be put in strict relationships with the complexation ability exhibited by CD towards different type of guest compounds. Moreover, based on what have observed on other water-sugars systems, it is reasonable to expect that the also the relaxation dynamics of hydrated CD may play a key role in their complexation activity. Finally, CD-water solutions are suitable model for studying complex bio-relevant processes (i.e. hydration and aggregation), strongly influenced by the formation and competition of HB involving water and organic molecules. Insights on HB arrangement and its cooperative reorganization as a function of temperature and solute concentration in CD-water solutions are achieved by exploiting the high capability of UV Raman and Brillouin scattering experiments, performed by taking advantage of the tuning of excitation sources of appropriate intensity of the synchrotron facility. The spectral changes in the Raman signals are used as vibrational signatures of the reorganization of HB network of water in the proximity of groups of CD [1]. In a complementary way, visible and UV Brillouin scattering experiments are implemented for measuring the collective dynamics of the system thus allowing to probe the characteristic timescale (0.1–10 ps) associated to the average timescale of the intermolecular bonds lifetime, typically observed in liquid HB systems [2]. The overall results presented here corroborate the potentiality of the joint use of inelastic scattering techniques to provide a comprehensive molecular view on the solvation dynamics in water-sugar solutions.

References

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