

### Thermodynamic hydration shell behaviour of cyclodextrin aqueous solutions

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Cyclodextrins (CDs) are natural cyclic oligosaccharides composed by a variable number of glucose units. Their characteristic truncated-cone shape permits to the CDs to behave as a molecular host able to encapsulate a wide variety of guest molecules which are poorly soluble in water. Water plays an important role in determining the complexation ability exhibited by CD towards different types of guest compounds since the molecular encapsulation capability of CD is directly related to the solvation properties of these complex sugars. Consequently, the investigation of hydration properties of CD molecules represents a very important topic and it is crucial for their application in different technological fields [1-3].

In this contribute, a joint combination of UV Raman and Brillouin scattering experiments have been used to investigate the structural dynamics of hydration water in aqueous solutions of natural and chemically modified cyclodextrins, as function of both temperature and solute concentration. In the Raman data analysis, the attention was focused on the changes occurring in the O-H stretching band of water. This spectral feature is in turn related to the structural rearrangement occurring in the H-bonding network of water molecules inside the hydration shell of CD. The ability of CD to form hydrogen bonds with water is expected to affect the ordered network of water-water hydrogen bonds in the solvent molecules placed around the solute. This "structure-breaker" effect on the tetrahedral H-bond pattern on water was investigated as a function of temperature, solute concentration and type of cyclodextrin, in order to correlate the extent of the destructuring effect induced by CD on surrounding water molecules with the different solubility exhibited by various kind of CD.

At the same time, information on the collective dynamics of the cyclodextrin-water solutions were provided by UV Brillouin scattering experiments. This technique gives the possibility to study liquid systems in the mesoscopic transfer region not accessible by other spectroscopic techniques. Its frequency window matches the water relaxation process time ( $\omega\tau \approx 1$ ), allowing us to probe the characteristic timescale 0.1–10 ps, which is associated to the average timescale of the intermolecular bonds lifetime, typically observed in liquid H-bond systems [4].

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-cyclodextrin solutions. All these knowledges could be used and useful to optimize the design of these natural nanocarriers.

#### References

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