

Introduction

Aqueous mixtures of carbohydrates and polyols play an important part in the majority of the formulation of food products (i.e in bakery, ice cream and sweeteners industries) and in several food processes.

The knowledge of physicochemical properties of such aqueous mixtures is mandatory for developing controlled and optimized processes.

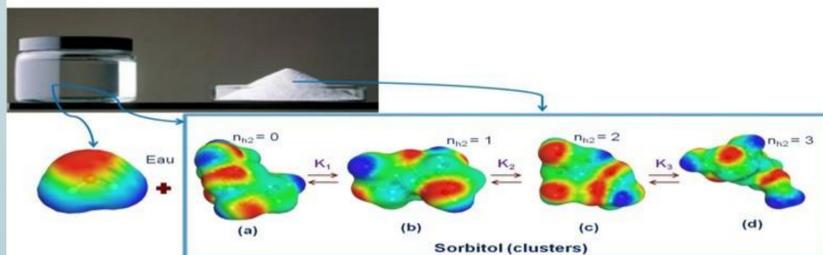
Raman spectroscopy has been intensively used experimentally since 1950 to investigate the behavior of bulk water [1,2], solid carbohydrates [3,4] and aqueous mixtures containing carbohydrates [5,6,7].

Today, simulation tools are able to compute Raman spectra of a custom molecule provided that the space arrangement of the atoms and bonds are given. This procedure allows us to compute Raman spectrum of one up to several molecules interacting with each other.

The most likely geometry can be found by making a link between computed and experimental data. Thus this geometry can be used to perform thermodynamics calculation (i.e COSMO-RS-PDHS model)[8].

The aim of this work is to use Raman spectroscopy to investigate **interactions between water and carbohydrates** (especially the hydration phenomena)

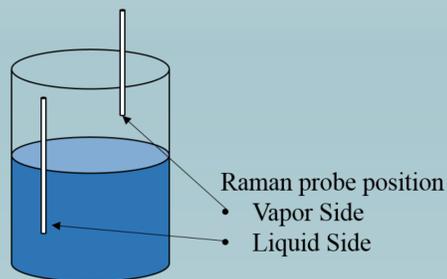
This poster presents preliminary results: Raman spectra of pure compounds (water, carbohydrates and polyols) and spectra of binary mixtures (water-carbohydrate, water-polyol).



Material and Methods

Experimental means:

The experimental Raman setup contains an 'in situ' Raman spectrometer supplied by ocean optics. The system includes a 532 nm laser beam, all Raman spectra have been recorded in the [50-4000]cm⁻¹ range using the in situ probe which allows us to take Raman spectra of liquid and gases both at Liquid-Vapor equilibrium.

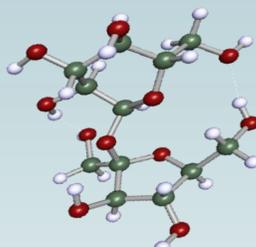


Simulation mean :

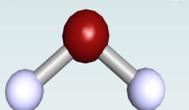
Our simulation tool is the TmoleX software which can be used to compute Raman spectra of compound of interest.

The procedure is listed below :

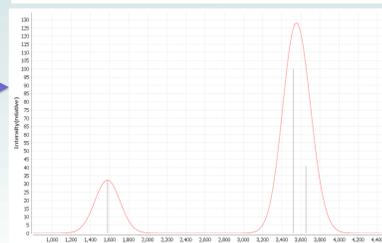
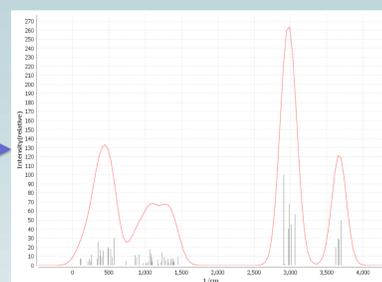
- Drawing of the desired geometry
- Energy calculation (DFT-RI + TZVP) with BP86 functional
- Computation of the vibrational frequencies (x-axis) and scattering cross sections (y-axis)



Exemple of a possible geometry of a sugar



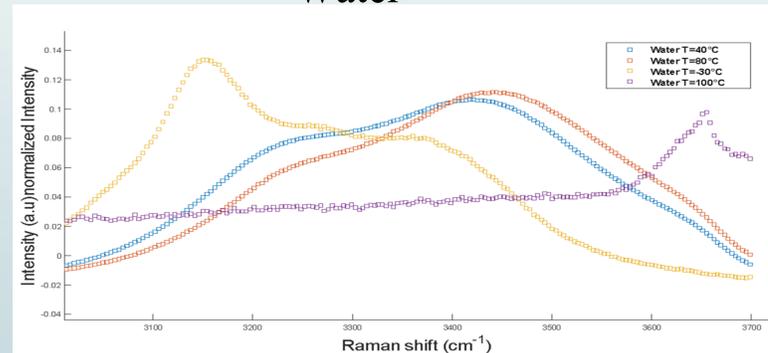
Exemple of a water molecule



Preliminary Results

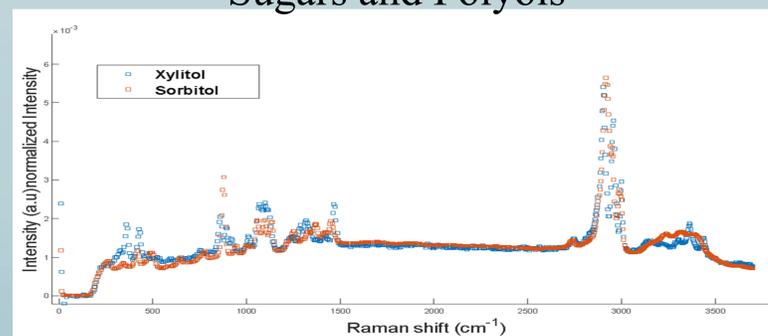
This poster aims to present preliminary results concerning experimental spectra of pure water in its different state (vapor, liquid, solid), solid carbohydrates and aqueous mixture of carbohydrate

Water



Raman spectra of ice at -30°C, liquid water at 40°C and 80°C and water at vapor/liquid equilibrium at 100°C are presented. Liquid water presents two very strong bands at 3220 cm⁻¹, 3435 cm⁻¹ and a weak band at 1600 cm⁻¹. Solid water reveals two strong bands at 3100 cm⁻¹ and 3400 cm⁻¹ whereas vapor water shows two weak bands at 1450 cm⁻¹ and 3645 cm⁻¹. As temperature increases, two strong bands of liquid water are shifted and the intensity of peak at 3200 cm⁻¹ decreases.

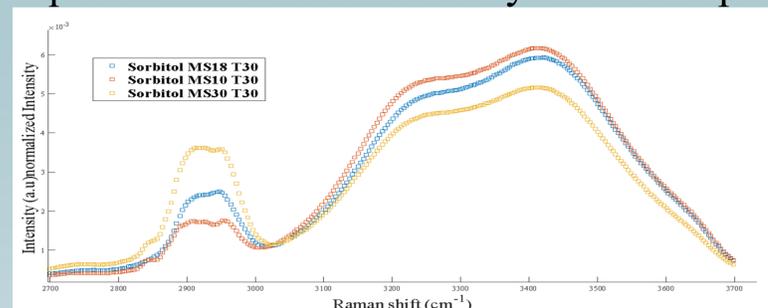
Sugars and Polyols



Unlike water, carbohydrates present weak shifts in the [500-1500] cm⁻¹, [3000-3600] cm⁻¹ range and strong shifts in [2700-2900] cm⁻¹ range. Like water, the [3000-3600] cm⁻¹ area allows the discrimination of solid/liquid carbohydrates and may be used to investigate the interactions between water and carbohydrates.

Fluorescence greatly impacts the measured Raman spectra and needs to be treated without altering the initial information provided by the Raman effect.

Aqueous mixtures of carbohydrates and polyols



Interactions between water-carbohydrate and water-polyol lead to modifications in the Raman spectra of mixture containing 30% of DS at 30°C

Raman spectra of aqueous mixtures containing respectively 10%, 18%, 30% DS of sorbitol are presented. As the weight ratio of carbohydrate increases, the intensity of the [2800-3000] cm⁻¹ spectral range (C-H band) increases and the intensity of the [3100-3500] cm⁻¹ region (O-H band) decreases.

The shift at 1600 cm⁻¹ occurs when liquid water is mixed with carbohydrates (Picture 5). However, Carbohydrates don't have bands in this spectral region, this information might be useful when searching for water content in such mixtures.

Conclusions

Raman spectroscopy detects structural modifications between the structure of pure compound such as water, carbohydrate-polyol and the structure of binary mixtures : water-carbohydrates, water-polyols.

Regarding pure water, these structural modifications are the consequence of a change of state. In the case of binary mixtures, the structural modifications are the result of water-carbohydrate and water-polyol interactions. Thus, Raman spectroscopy appears as a promising tool to investigate the hydration phenomena regarding carbohydrates and polyols.

Bibliography

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