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Host-guest complexes between beta-cyclodextrins and small drugs for SERS detection in drinking water

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beta-CycloDextrin (b-CD) is a macrocyclic oligosaccharide composed of seven D-glucopyranoside units linked in alpha-(1,4) bonds. b-CD has a truncated cone tri-dimensional structure. Its central cavity is hydrophobic, allowing low-polarity molecules to be encapsulated partially or entirely by host-guest interaction, meanwhile the external part is hydrophilic because of the presence of 21 hydroxyl groups making b-CD soluble in water. This host-guest type relationship can modify the physical, chemical or biological characteristics of the guest molecule, and applications are found in practically all sectors of industry. One of these applications consists in functionalizing silver nanoparticles with b-CD-SH in order to develop a Surface-Enhanced Raman Scattering (SERS) sensor to detect pollutants such as PAHs [1]: the b-CD cavity traps PAHs near the metallic surface where the large increase in Raman cross-section is induced. Such a SERS sensor could be considered for the detection of traces of small drugs (salicylic acid, paracetamol) in drinking water. That is why we have started to study host-guest complexes between salicylic acid or paracetamol with b-CD.
The advent of soft ionization techniques has allowed for extensive examination of cyclodextrin complexes by mean of mass spectrometry, and structural information on b-CD complexes have recently been provided by IRMPD and IM spectroscopy [2] or also action-FRET [3]. Our goal is to probe in the gas phase the relative position of the non-covalently bound subunits in two systems: complexes between salicylic acid and b-CD and complexes between paracetamol and b-CD. These structures are obtained by combining IRMPD spectroscopy experiments and quantum calculations for simulating IR spectra on mass-selected ions. Comparison with studies in the condensed phase will give information on the possible conversion of inclusion complexes to nonspecific complexes (and vice versa) and on the importance of relative interactions for the formation of the complexes.
We have started to extend these studies to different molecular cages, more precisely gamma-cyclodextrin (eight glucopyranose units) and methylated beta-cyclodextrins : the degree of methylation should modify characteristics such as complex formation, toxicity and solubility for the included guest molecule [4].

[1] Tijunelyte et al. Environ. Sci. Pollut. Res., 24, 27077-27089 (2015).
[2] J.U. Lee et al. Molecules 25, 4048 (2020).
[3] Q. Duez et al. New J. Chem. 41, 41, 1806 (2017).
[4] Fenyvesi et al. J. Pharm. Sci. 103, 1443-1452 (2014).

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