Studying the properties of PAH and hydroxylated PAH in interaction with water in the context of laboratory astrophysics

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Polycyclic Aromatic Hydrocarbons (PAHs) and water molecules are ubiquitous in regions of star and planet formation in which they have an important contribution to the chemical evolution [1,2]. In cold and dense regions, water molecules can adsorb on icy and carbonaceous grains containing PAHs. The irradiation by energetic photons or particles (cosmic rays) may lead to the formation of strongly bounded PAH-water complexes. The latter species correspond to the incorporation of oxygen into PAH by the formation of the carbonyl (C=O) or hydroxyl (C-OH) function leading to ketones, quinones, enols or alcohols [3,4,5] which are key molecules in prebiotic chemistry. Exposure of the icy grains to UV irradiation may then lead to the evaporation of these new species or to weakly bounded clusters made of PAH, functionalized PAH and water [6]. Therefore, studying PAH-water systems in the laboratory by experiments and/or quantum chemistry is needed to better understand the role and the survivability of such molecular systems in these regions in order to support astronomical observations.

We are investigating such topics thanks to a strong collaboration between three laboratories in Toulouse (IRAP, LCAR and LCPQ). This has led us to develop different methodologies to study mixed PAH-water systems. I will focus on the combined experimental techniques which permit us to produce, manipulate, isolate and study such species [7,8] and our recent results which deal with hydroxylated PAHs (OH-PAHs) mixed with water. Our general methodology is to use sources which generate cationic PAHs that act as nucleation seeds for a further aggregation with the surrounding molecules (water or PAH) at low temperature. The formed clusters/complexes are either excited with collisions or photons. The induced modifications are observed by mass spectrometry techniques. These measurements allow us to quantify relevant parameters for astrochemistry such as the dissociation energies, the IR spectra or the collision/photon cross-sections of these species. Besides, these studies give insights on fundamental processes such as photo-excitation and energy redistribution which are at play in astrophysical environments and may be of interest for atmospheric chemistry [9,10].

I will focus my presentation on recent results obtained with the “Agrégats” setup at LCAR and the “FELion” setup at FELIX on the 1-hydroxypyrene (OH-Pyr) and 1-hydroxyphenanthrene (OH-Phen) in interaction with water. These results are obtained either by collision induced dissociation or IR tagging spectroscopy [11]. They demonstrate that OH-PAHs have a specific interaction with water through the hydroxyl function and a higher dissociation energy than the bare PAH. Additionally, the modification of the IR spectrum induced by one water molecule in interaction with $OH\text{-}PAH^+$ is discussed, in particular regarding the expected OH wagging modes around 1000 cm-1 that were not observed experimentally. These studies question isomerization mechanism and the anharmonic couplings in such systems. Finally, I will present the ongoing development in LCAR regarding the “CASSOULExp” setup which aim to systematically perform IR tagging spectroscopy on complexes made of several functionalized or bare PAHs and water molecules.

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