Master student internship proposal

Laboratory	Laboratoire Collisions Agrégats Réactivité
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Title	**Collision induced dissociation of complexes carbonaceous molecular systems of astrophysical interest**
Keywords	molecular physics, collision, cluster physics, mass spectrometry, astrochemistry,
Required skills	**Very good educational background in physics and physical chemistry** (quantum physics, molecular physics, electromagnetism, optics, electronics) and **strong interest and skills in experimental physics and data analysis**. Knowledge in astrochemistry and astrophysics are a not mandatory but will be appreciated. *Feel free to contact us if you like the topic even if your skills are not perfectly in line with the internship!*
Techniques methods in use	Cluster source, ion optics, filter, mass spectrometry, collision induced dissociation, cryogeny
Possibility of a PhD	Yes, funded by the french ANR **CASSOULExp project**.

Cosmic nanograins play key roles in the physical and chemical evolution of the interstellar medium. Indeed, these nanosized catalytic platforms can interact with molecules of the gas phase (e.g. H_2O, CO, etc.), through adsorption and desorption processes, which can result in the production of new species that chemically enrich star and planet forming regions. We are especially interested in carbonaceous nanograins made of polycyclic aromatic hydrocarbon (PAH) molecules and their derivatives [1]. In presence of water and UV photons, PAHs are expected to be oxidized, thus forming alcohol or ketone molecules [2,3] which are of prebiotic interest.

During two previous beamtimes, the first at the SOLEIL synchrotron and the second at the ILM laboratory, we have studied PAH-water cationic complexes with different experimental setups in order to explore their dissociation properties (fragmentation channels, energetics and dynamics). These setups were equipped with an ion trap capable of performing collision induced dissociation (CID) at controlled collision energy that allows to measure the fragmentation channels of a parent species as a function of the internal energy injected into it. In particular, we could study CID of the pyrene-water cationic complex ($[(C_{16}H_{10}):OH_2]^+$) and its dehydrogenated form ($[(C_{16}H_9)OH_2]^+$) and the 1-hydroxypyrene cation ($[C_{16}H_9OH]^+$) and its hydrogenated form ($[HC_{16}H_9OH]^+$). Despite their similar compositions and structures, the raw CID data of these molecular systems are very different and show fragmentation pathways which are specific to each species.

The aim of this internship will be to analyze the CID data obtained during the two beamtimes in order to shed light on the fragmentation pathways of these complex systems and to better interpret the observed differences. Additionally, the student will have the opportunity to use the Agrégat setup in LCAR [4] (see **Figure 1**) to further investigate fragmentation [5,6] or adsorption [7] processes on PAH-water cationic clusters made of hydroxypyrene ($C_{16}H_9OH$), which is a good analogue of the species studied at SOLEIL or ILM. Thus, these new measurements will be compared to the one of the two beamtimes to better understand the mechanisms at play. Depending on the internship duration and the student involvement and interest, she/he will then perform threshold CID measurements with this experimental setup in LCAR and/or he/she will also build a statistical model that will help to extract dissociation energies and rates.

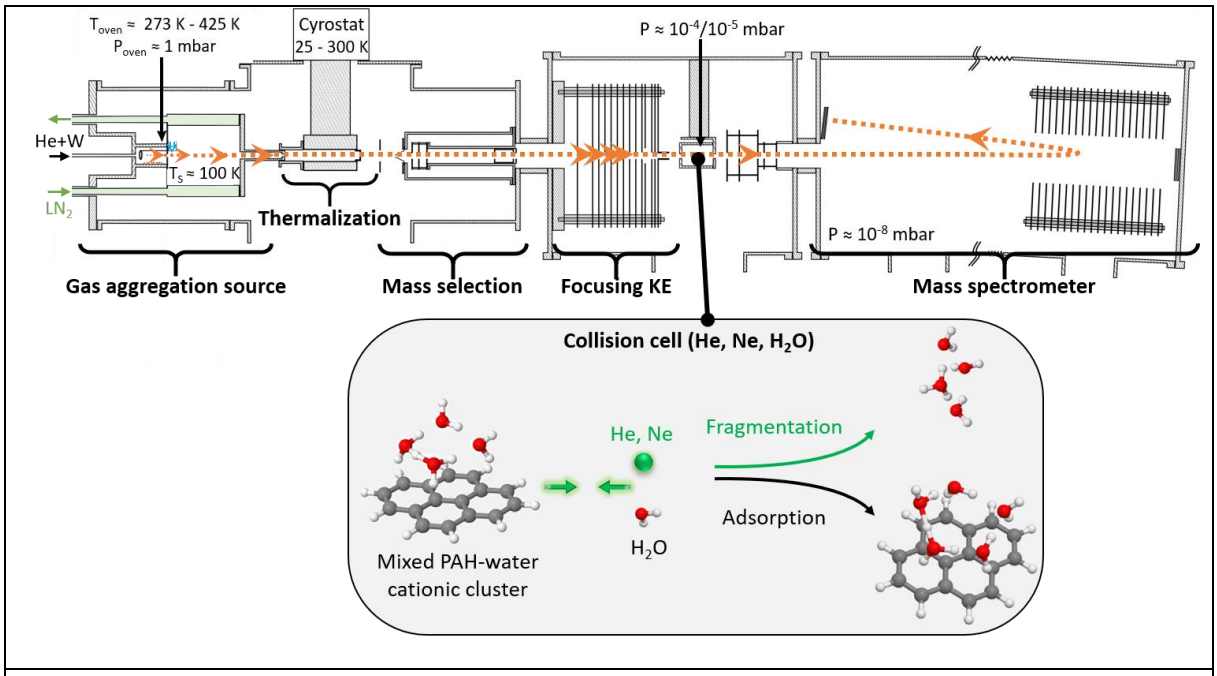


Figure 1. Working principle of the "Agrégats" setup. Cationic molecular cluster are generated by a source and thermalized down to 25 K. They are mass-selected and focused in kinetic energy (KE) into a cell containing rare gas (He, Ne, etc..) or small molecules (e.g. H_2O) to reach a single collision regime. Depending on the kinetic energy in the center of mass, fragmentation or adsorption can occur in the collision cell. The products are analyzed by a mass spectrometer in reflectron-ToF configuration. Hence, the two processes can be studied as a function of the KE.

Bibliography

[1] Pilleri, P. *et al. A&A* **542**, A69 (2012).

[2] Bernstein, M. P. *et al. Science* **283**, 1135-1138 (1999).

[3] Bouwman, J. *et al. A&A* **511**, A33 (2010).

[4] Braud, I. *et al. Rev. Sci. Instr.* **88**, 043102 (2017).

[5] Zamith, S. *et al. J. Chem. Phys.* **153**, 054311 (2020).

[6] Nair, A. M. *et al. Phys. Chem. Chem. Phys.* **26**, 5947-5961 (2024).

[7] Zamith, S *et al. J. Phys. Chem. A.* 130 (39), 7852 (2026).