Master student internship proposal

Laboratory	Laboratoire Collisions Agrégats Réactivité
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Title	**Infrared spectroscopy of carbonaceous nanograins for astrochemistry**
Keywords	molecular physics, spectroscopy, cluster physics, mass spectrometry, optics, 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 guide, filter and trap, mass spectrometry, cryogeny, OPO laser, action spectroscopy
Possibility of a PhD	Yes, funded by the french ANR **CASSOULExp project.**

In the interstellar medium (ISM), cosmic grains are crucial for its chemistry. Indeed, these catalytic platforms interacts with molecules of the gas phase and produces new species which chemically enrich star and planet forming regions. In some regions of the ISM, it exists an abundant population of grains which have a (sub-)nanometer size, also called nanograins. Since they have a huge surface over volume ratio, nanograins are at play in the physical and chemical evolution of these regions. Microscopically, they correspond to atomic or molecular clusters down to single molecules of polycyclic aromatic hydrocarbon (PAH) [1]. The nanograin morphology especially drives the fundamental interactions (adsorption, desorption, molecular diffusion) between them and small molecules of the gas phase (e.g. H_2O, CO, etc.). Therefore, the understanding of nanograin structures is a crucial step which remains very little explored up to now [2].

The CASSOULExp setup (see **Figure 1**) has been developed in the framework of an ANR project [3] which aims to study gas-nanograin-photon interaction in astrophysical conditions. This setup is equipped with a molecular cluster source to produce the nanograins and a cryogenic ion trap to store them in extreme isolation conditions (~6 K, ~10^{-9} mbar). The aim of this internship is to couple this setup to a tunable IR laser source (IR OPO) and to perform the first IR spectra on mixed PAH-water clusters. The setup will then be used to systematically characterize the structures of cationic carbonaceous nanograins (e.g. PAH_n^+ or $[PAH_n(H_2O)_m]^+$, [4]). The student will participate to this development and perform measurements of IR action spectra of some simple clusters to validate the methodology. Depending on the internship duration and the student involvement and interest, she/he will also perform more measurements on more complex nanograins and study the modification of these spectra as a function of the nanograin composition. Moreover, these results will be compared to quantum chemistry calculations, performed by our collaborators at LCPQ, in order to evaluate the nanograin structures [5]. These new data will notably help to interpret astrophysical observations which are currently performed by the James Webb Space Telescope [6].

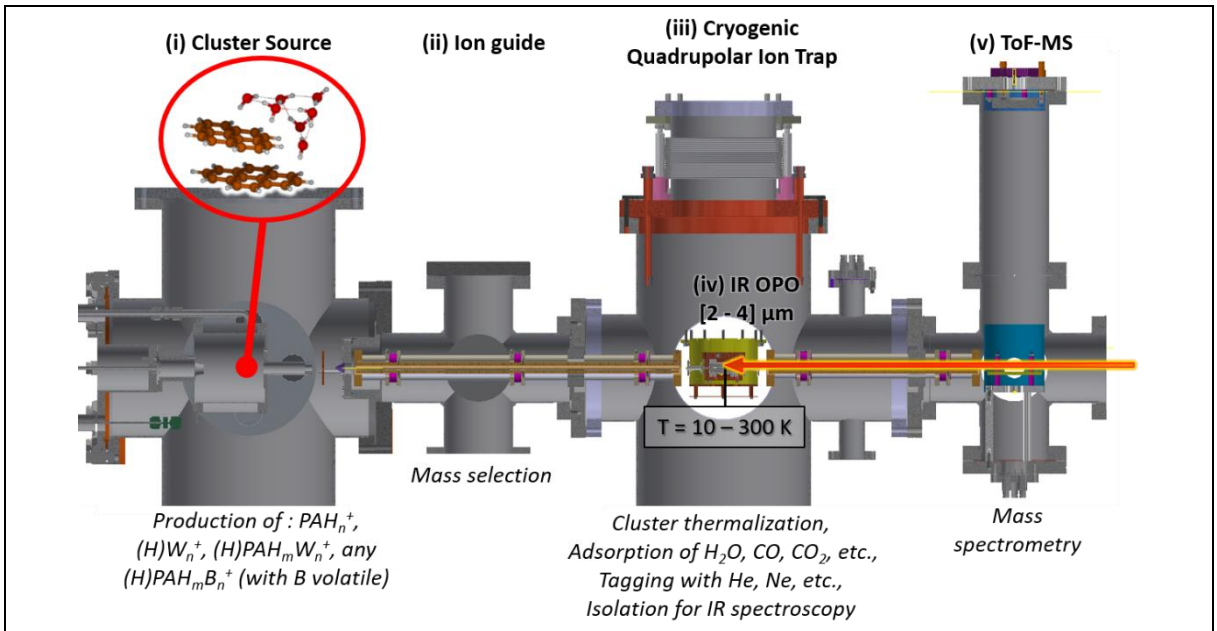


Figure 1. Working principle of the CASSOULExp experiment. Nanograins are (i) produced by the molecular cluster source, then they are (ii) guided, mass-selected and (iii) stored in a cryogenic ion trap where tagging with rare gaz (Ne, Ar) or adsorption of further small molecular species (H_2O, CO, etc…) can occur. (iv) Irradiation of the trapped species is performed with an IR OPO (optical parametric oscillator) and the irradiated species are (v) analyzed by an orthogonal time-of-flight mass spectrometer (ToF-MS). From such measurements, we can obtain the IR action spectra of the studied nanograins as a function of the experimental conditions: number of monomers (N), number of additional water molecules (N_W), etc.

Bibliography

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

[2] Chatterjee, K. *et al. Chem. Sci.* **9**, 2301 (2018).

[3] Marciniak, A. *et al. hal-03752080*, https://hal.archives-ouvertes.fr/hal-03752080.

[4] Zamith, S. *et al. J. Phys. Chem. A* **126**, 3696-3707 (2022).

[5] Dontot, L. *et al. J. Phys. Chem. A* **123**, 9531-9543 (2019).

[6] Berné, O. *et al. PASP* **134** (1035), 054301 (2022).