







GAS PHASE ACTION SPECTROSCOPY OF DE-HYDROGENATED METHYL-PYRENE CATIONS STORED IN ELECTROSTATIC ION STORAGE RING

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IN COOPERATION WITH :	iLM
LEVEL :	M2
TEAM(S) :	SPECTROBIO
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KEYWORD(S):

SCIENTIFIC CONTEXT :

Electrostatic ion storage rings (e.g. Mini-Ring at ILM, DESIREE in Stockholm) allow for the study of molecular processes over a wide range of time scales (from microseconds to tens of minutes), including dissociation, ionization, fluorescence, radiative cooling, etc. PAHs (polycyclic aromatic hydrocarbons) are systems encountered in astrophysics in the interstellar medium, where they are subjected to various types of radiation that can induce the processes mentioned above, but also rather rich chemistry certainly



involving isomerization processes. These electrostatic storage rings allow studies on these molecules in conditions close to those of the interstellar medium such as, e.g., very high vacuum, very low temperature, long observation times.

The branching ratios between the different relaxation processes as well as the associated lifetimes are very dependent on the internal energy of the system as well as on possible isomerization processes. In experiments concerning the radiative cooling of PAHs (either ours or those of competing groups), the recurrent question of isomerization has often been eluded and, as a consequence, has not been sufficiently well treated until now. The internship will focus on the particular case of the dehydrogenated methyl-pyrene ion (C17H11+) which presents two isomers: one with a methylene group (C16H9-CH2)+, the other with a tropylium ring with 7 carbon atoms.

MISSIONS:

PAHs with methyl groups, such as methyl-pyrene, are expected to be present in some astrophysical environments although they are more fragile than non-substituted PAHs. The unimolecular dissociation of methyl-pyrene by emission of a hydrogen atom leads to two possible isomers: one with a CH2 methylene group, the other with a tropylium-like structure including a C7 heptagonal ring. These two species having different absorption spectra in the visible and UV should be clearly identifiable experimentally. Experiments have been performed very recently at iLM on Mini-Ring and in Stockholm on DESIREE. The trainee will perform data analysis to study the possible formation of these isomers initially in the ion source and the competition between radiative relaxation, dissociation and isomerization. If necessary, the trainee will perform complementary experiments on Mini-Ring in order to complete or refine the experimental data set.

This internship will possibly open to a thesis.

BIBLIOGRAPHY :

J. Bernard, et al., Experimental and theoretical study of photo-dissociation spectroscopy of pyrene dimer radical cations stored in a compact electrostatic ion storage ring, Phys. Chem. Chem. Phys. (2021) 10.1039.D0CP05779G. https://doi.org/10.1039/D0CP05779G

M.H. Stockett, et al., Unimolecular fragmentation and radiative cooling of isolated PAH ions: A quantitative study, J. Chem. Phys. 153 (2020) 154303. https://doi.org/10.1063/5.0027773.