

Disentangling isomers in collision induced dissociation of PAHs

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The AROMA (Astrochemistry Research of Organics with Molecular Analysis) setup [1] has been designed to analyse the organic molecular content of cosmic dust analogues, as part of the NANOCOSMOS ERC project. In this work, we test the capabilities of AROMA to discriminate structural isomers of polycyclic aromatic hydrocarbons (PAHs) using a Collision Induced Dissociation (CID) scheme.

AROMA is an hybrid setup, composed of a laser desorption/ionization source, coupled with a Linear Quadrupole Ion Trap (LQIT) and an orthogonal Time Of Flight (oTOF). Controlled CID experiments are performed in the LQIT under various conditions of colliding Ar gas pressure and Dipolar Excitation (DE) conditions.

We present results obtained for the pyrene (PYR) cation $C_{16}H_{10}^+$ and two of its isomers, ethynyl-phenanthrene (ETHPH) and fluoranthene (FLU), all at mass $m/z=202.08$. We explored the influence of the DE parameters (amplitude, frequency, duration of the DE). We focus here on conditions that we consider as the most promising to discriminate isomers. From the breakdown curves giving the dissociation yield as a function of the excitation time [0, 1500] μs , we derived a time value at 50% dissociation for each case [2]. This value differs significantly between ETHPH and the other isomers. On the other hand, we studied branching ratios and show that the C_4H_x/C_2H_x branching ratio can be used to disentangle FLU from the other isomers.

Perspectives will be given on the analysis of complex mixtures including meteorite samples.

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References

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