



SEMINAIRE ISMO

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Electronic Spectra of Aromatic Hydrocarbons: A Deductive Approach to the Diffuse Interstellar Bands

The diffuse interstellar bands (DIBs) are a series of more than 500 interstellar absorption features, first observed in 1919. After almost a century of experimental and theoretical investigation, the first and only identified carrier of DIBs, C_{60}^+ , was identified late last year.

In order to determine which aromatic chemical species are likely to be carriers of the DIBs, spectroscopic features of small polycyclic aromatic hydrocarbon (PAH) species with chromophores ranging from 6 to 17 carbon atoms were studied spectroscopically and theoretically. Trends are explored for classes of PAH with differing charge states and multiplicities, for multiple electronic transitions. The transitions observed include the $D_1 \leftarrow D_0$ transitions of neutral PAH radicals and radical cations as well as strong transitions to higher excited states of PAH radicals and radical cations.

This presentation will introduce the spectroscopic techniques used in this study for recording electronic spectra of molecules in a simulated interstellar environment. The spectra obtained will then be discussed in light of *ab-initio* and semi-empirical TD-DFT methods. Trends in the spectroscopic properties of the molecules observed will be used to predict the spectral properties of larger PAH molecules that are experimentally difficult to directly observe in the gas-phase.

As a result of the work presented, several classes of PAH can now be largely dismissed as possible carriers of the DIBs. The implications of this work and the future direction of research into the longest unsolved mystery in astronomy will be discussed.

Mardi 5 avril 2016 à 11h
Bât. 210 – Amphi 1 (2^{ème} étage)
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