Improving potential energy surfaces for *in silico* spectroscopic studies of PAHs of astrophysical interest

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Abstract: Polycyclic Aromatic Hydrocarbons (PAHs) are a family of organic compounds composed of aromatic rings of carbon atoms, whose peripheral valencies are saturated by hydrogen atoms. PAHs (or closely related species) are thought to be the carriers of the so-called Aromatic Infrared Bands (AIBs) at ∼3.3, 6.7, 7.7, 8.6, 11.3 μm. These features are among the strongest emission features observed in the interstellar medium in the infrared (IR), and present some interesting variability from one observed source to another. Therefore, the IR spectroscopy of PAHs is of paramount importance in astrophysics and astrochemistry: A better understanding of it, is essential to infer from IR observations, informations about PAHs composition and physical parameters of their environment [1].

In our laboratory, we have developed a computer code, CONVIV, which solves the Schrödinger equation for molecular vibrational degrees of freedom with state-of-the-art accuracy [2, 3]. It can be used to perform calculations of the infrared spectrum of molecules of arbitrary sizes. The internship will consist in using the CONVIV code to compute and interpret theoretically, the IR spectra of selected members of the PAH family.

CONVIV uses as input data an *ab inito* a potential energy surface (PES). Quartic Force Fields (QFFs) are tractable and convenient means by which one can describe PESs of medium-size molecular systems. For many PAHs, there are QFFs available in the literature. However, these fourth order truncated force fields can produce PESs diving artefactually to $-\infty$, when negative force constants are present. Moreover, they are not accurate enough for the interpretation of the most recent astrophysical observations, in particular those from the James Webb Space Telescope (JWST) or from the MATISSE instrument operating at the Very Large Telescope Interferometer (VLTI) of the European Southern Observatory (ESO). A possible workaround to these issuee investigated in this internship will be to replace the quartic Taylor expansion along the vibrational modes of the molecules by more adapted functional form of potentials (Kratzer potential for vibrational modes carrying the totally symmetric representation and trigonometric Pöschl-Teller for other modes).

Prérequis: Basis of quantum mechanics and spectroscopy, computational skills (Fortran and Python).

References

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[3] P. Cassam-Chenaï, Y. Scribano and J. Liévin, Chemical Physics Letters **466**, 16-20 (2008).