High Resolution Spectroscopy of PAHs and Derivatives Using a Room Temperature Long Pathlength Cell and the Jet-AILES Experiments

S. Gruet[a,b], O. Pirali[a,b], M. Goubet[c], T. R. Huet[c], R. Georges[d], P. Soulard[e], and P. Asselin[e]

[a] Institut des Sciences Moléculaires d'Orsay, UMR8214 CNRS, Bât. 210, Université Paris-Sud, 91405 Orsay Cedex, France, Tel : + 33 1 69 35 81 72, E-mail : sebastien.gruet@synchrotron-soleil.fr

[b] Ligne AILES, synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin, BP 48, 91192 Gif-sur-Yvette, France, Tel : + 33 1 69 35 97 42, E-mail : olivier.pirali@synchrotron-soleil.fr

[c] Laboratoire de Physique des Lasers, Atomes et Molécules, UMR 8523 CNRS, Bât. P5, Université Lille 1, 59655 Villeneuve d'Ascq Cedex, France, Tél : +33 3 20 33 64 60, E-mail : manuel.goubet@univ-lille1.fr; E-mail : therese.huet@univ-lille1.fr

[d] Institut de Physique de Rennes, UMR 6251 CNRS, Bât. 11C, Campus de Beaulieu, Université de Rennes 1, 35042 Rennes Cedex, France, Tel : + 33 2 23 23 67 53, E-mail : robert.georges@univ-rennes1.fr

[e] Laboratoire Dynamique, Interactions et Réactivité, UMR 7075 CNRS, Université Pierre et Marie Curie, 4 place Jussieu, F-75252 Paris Cedex 05, France, Tel : +33 1 44 27 30 25, E-mail : pascale.soulard@upmc.fr; E-mail : pierre.asselin@upmc.fr

Polycyclic Aromatic Hydrocarbons (PAHs) have long been suspected to be the carriers of so called Unidentified Infrared Bands (UIBs) [1,2]. A better understanding of the carriers's nature of these broad and unresolved emission features requires an extensive range of experimental and theoretical studies. Most of the results published in the litterature report rotationally unresolved spectra of pure carbon as well as heteroatom-containing PAHs species in different conditions (phase, temperature, degree of ionization state and of hydrogenation, ...). To date, high resolution measurements reporting rotational structure of the IR/FIR vibrational bands are very scarce.

Recently, several high resolution gas phase absorption techniques enabled to rotationally resolve the IR and FIR bands PAHs such as naphthalene [3] and pyrene [4]. At SOLEIL, synchrotron-based high resolution FT spectroscopy using both room temperature long absorption cell and a continuous supersonic jet experiment provided the first rotationally resolved spectra of several FIR bands of relatively large C-bearing molecules [5].

We report the rotational analysis of the most intense c-type bands in the 50-600 cm^{-1} range of several two rings PAHs and the spectra of larger species under jet-cooled conditions.

The experimental rovibrational parameters were obtained with the help of anharmonic DFT calculations. The Jet-cooled spectra have evidenced hot band sequences involving the low frequency vibrational modes, shading some light on their contributions to the confused unresolved Q-branch at room temperature. The rotational analysis of these IR/FIR bands might help to search these species in space and to model the IR emission responsible for the UIBs.

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