ROTATIONAL STRUCTURE OF THE IR/FIR BANDS OF SMALL PAHS

O. PIRALI[a], S. GRUET[a], M. VERVLOET, *Ligne AILES, Synchrotron SOLEIL, L'Orme des Merisiers Saint-Aubin, 91192 Gif sur Yvette Cedex - France*; M. GOUBET, T. R. HUET, *Laboratoire de Physique des Lasers, Atomes et Molécules, UMR 8523 CNRS - Université Lille 1, Bâtiment P5, F-59655 Villeneuve d'Ascq Cedex, France*; R. GEORGES, *Université de Rennes 1, Institut de Physique de Rennes, CNRS, UMR 6251, F-35042 Rennes Cedex, France*; P. SOULARD, P. ASSELIN, *UPMC Université Paris 06, UMR 7075 CNRS, Laboratoire de Dynamique, Interactions et Réactivité (LADIR), F-75005, Paris, France*.

Accurate spectroscopic measurements in the laboratory of PAH molecules are required to better understand their excitation/relaxation processes which could be responsible for the Unidentified Infrared Bands observed in various objects in space. In particular very few is known concerning the rotational structure of the IR/FIR bands of PAHs. We used the high resolution Fourier Transform interferometer of the AILES beamline of synchrotron SOLEIL to record the rotationally resolved spectra of several IR/FIR vibrational modes of naphthalene ($C_{10}H_8$) and its derivatives: quinoline (C_9H_7N), isoquinoline (C_9H_7N), azulene ($C_{10}H_8$), quinoxaline ($C_8H_6N_2$), quinazoline ($C_8H_6N_2$). Firstly, the intense band associated with the ν_{46} CH bending out of plane mode of naphthalene recorded under jet conditions (Jet-AILES experiment developed on the AILES beamline by the IPR-LADIR-PhLAM consortium) revealed transitions involving low J and Ka rotational quantum numbers. These new data permitted to accurately fit the ground state rotational constants and to improve the ν_{46} band constants[b]. As a second step, we performed the rotational analysis of the low frequency ν_{47} and ν_{48} bands of naphthalene recorded at room-temperature in the long absorption pathlength cell from ISMO. As a last step, the high resolution spectra of several bands of azulene, quinoline, isoquinoline and quinoxaline were recorded at room temperature and analyzed using the same procedure. All the rotational constants fitted in the present work were compared to the results of anharmonic DFT calculations realized at various levels of accuracy.

[a] Also at: Institut des Sciences Moléculaires d'Orsay, UMR 8214 CNRS-Université Paris-Sud, Bât. 210, 91405 Orsay cedex, France.

[b] S. Albert, et al.; Faraday Discussions, **150**, 51 (2011)