High Resolution Microwave and Infrared Spectroscopy Supplemented by Anharmonic DFT Calculations as Tools for the Structural Determination of Two Di-aza-naphthalene: [1,5]- and [1,6]-naphthyridine.

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The unidentified infrared bands (UIBs) observed in most classes of astrophysical sources [1] are strongly suspected to be carried by polycyclic aromatic hydrocarbons (PAHs). The hypothesis of N-bearing PAHs occurring in the ISM has been considered since nitrogen is the seventh most abundant element in the universe. Moreover, because of their higher permanent dipole moment, PANHs are an interesting class of complex aromatic hydrocarbon molecules since they can be detected by microwave spectroscopy more easily than non-polar unsubstituted PAHs [2]. To date, high resolution measurements reporting rotational structure of the infrared (IR) vibrational bands are very scarce. Recently, some high resolution techniques provided interesting new results to rotationally resolve the IR and far-IR bands of these relatively large carbonated molecules of astrophysical interest. One of them is to use the bright synchrotron radiation as IR continuum source of a high resolution Fourier transform (FTIR) spectrometer [3].

We report in this poster the analysis of the pure rotation spectrum of [1,6]-naphthyridine recorded in the 4-20 GHz range using the Fourier transform microvawe (FTMW) spectrometer in Lille. The obtained molecular parameters in the ground vibrational state were then used to analyze the ν_{38}-0 (~483 cm^{-1}) and ν_{34}-0 (~842 cm^{-1}) rovibrational bands recorded using the high resolution FTIR spectrometer of the AILES beamline at the synchrotron SOLEIL. In addition, the ν_{22}-0 (~166 cm^{-1}) and ν_{18}-0 (~818 cm^{-1}) rovibrational bands of [1,5]-naphthyridine (centrosymmetric isomer without permanent dipole moment) have been analyzed. For both isomers, the set of experimental rotational constants was used to correct the calculated rotational constants at equilibrium, from which a pseudo-experimental equilibrium structure has been estimated.

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