FAR-INFRARED SPECTRUM OF CYCLOHEXANE FROM SOLEIL SYNCHROTRON SOURCE

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Cyclohexane (C_6H_{12}) is a well-known species in chemistry and it is commonly used as apolar solvent in several applications. Due to the lack of permanent dipole moment, pure rotational transitions of cyclohexane cannot be observed. The determination of its molecular geometry in the isolated environment of the gas phase is still challenging and the best structure reported in the literature is based on isotopic substitution[1] (r_s). Still, a way to access the ground state rotational constants (B_0) of cyclohexane, is provided by Raman[2] and infrared (IR) spectroscopy. The latter technique was recently used to study the vibrational excited states of cyclohexane[3] between 1100 to 4000 cm^{-1}. However, the ro-vibrational analysis of the cyclohexane fundamentals is not complete as the two IR active modes (ν_{32} and ν_{16}), located in the far-infrared (FIR) region, have never been observed. Indeed, these two bands of cyclohexane are predicted as very weak in intensity and the corresponding high-resolution spectra were obtained using the synchrotron radiation available at the AILES beamline of SOLEIL. First, a weak band centered at around 520 cm^{-1} was observed, which was safely assigned to the ν_{16} fundamental band. Using literature data in combination with *ab initio* parameters as guideline, about 3500 transitions were assigned. The data obtained from this fit were then used to identify the $\nu_{32} + \nu_{16} - \nu_{32}$ hot band, and other hot bands that are currently under investigation. These results and those involving the lowest band at about 240 cm^{-1} (ν_{32}) will be illustrated and combined with the other data of the literature, thus providing a full characterization of the IR spectrum for cyclohexane.

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