First rovibrational signatures of cyclic $(HF)_3$ in the far infrared region.

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Since its first setting-up in 2009, the Jet-AILES apparatus has evolved toward a sensitive infrared broadband probe relevant for a variety of gas phase molecular systems. This set-up combines a supersonic free jet to the high resolution FTIR spectrometer equipping the AILES beamline of the synchrotron light source SOLEIL. A series of slit nozzles up to 90 mm length, heatable up to 473 K, are used to produce seeded supersonic planar expansions from gaseous, liquid or solid samples to form small molecular clusters at rotational temperatures in the 20-30 K interval.

The capabilities of Jet-AILES are highlighted through some recent results obtained so far in the field of weak interactions within small molecular clusters. Several rovibrational signatures of intermolecular modes within hydrogen bonded complexes bearing HF have been detected in the far infrared region : the fully resolved jet-cooled spectrum of both in-plane ν_6 and and out-of-plane ν_4 bending modes of cyclic $(HF)_3$ trimer have been recorded up to 0.005 cm^{-1} resolution. The rovibrational analysis of such low frequency intermolecular modes provides reliable data about their structure and vibrational dynamics. The absence of permanent dipole moment of cyclic $(HF)_n$ clusters prevents their study using MW spectroscopy. Moreover, intramolecular vibrational redistribution causes large homogeneous broadenings in the HF donor stretch mode spectrum of $(HF)_3$. As a matter of fact, far infrared absorption jet spectroscopy appears as the only possibility to bring a definite answer about the vibrationally averaged structure of $(HF)_3$ [1].

Ground and upper states parameters of $(HF)_3$ have been obtained using a global fit of 246 IR transitions of both ν_6 and ν_4 bands. The rotational parameters derived from our spectroscopic fit clearly provide reliable structural information: firstly the vibrationally averaged planarity of cyclic $(HF)_3$, also supported by a very small value of the inertia defect, secondly the slight weakening of the hydrogen bond in the intermolecular states evidenced from the center of mass separations of the HF constituents determined in the ground, $v_6=1$ and $v_4=1$ states of $(HF)_3$ as well as the negative variation of fitted rotational constants upon excitation.

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