

THE JET-COOLED HIGH-RESOLUTION IR SPECTRUM OF FORMIC ACID CYCLIC DIMER

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As the simplest carboxylic acid, formic acid (FA) is an excellent model molecule to investigate the general properties of carboxylic acids. FA is also an atmospherically and astrophysically relevant molecule. It is well known that its dimeric form is predominant in the gas phase at temperatures below 423 K.^a The cyclic conformation of the dimer (FACD) is an elementary system to be understood for the concerted hydrogen transfer through equivalent hydrogen bonds, an essential process within biomolecules. The IR range is a crucial spectral region, particularly the far-IR, as it gives a direct access to the intermolecular vibrational modes involved in this process. Moreover, due to its centrosymmetric conformation, the FACD exhibits no pure rotation spectrum and, due to spectral line congestion and Doppler broadening, IR bands cannot be rotationally resolved at room temperature.^b So far, only parts of the ν_5 -GS band (C-O stretch) have been observed under jet-cooled conditions using laser techniques.^c

We present here six rotationally resolved IR bands of FACD recorded under jet-cooled conditions using the Jet-AILES apparatus and the QCL spectrometer at MONARIS, including the far-IR ν_{24} -GS band (intermolecular in-plane bending). Splitting due to vibration-rotation-tunneling motions are clearly observed. A full spectral analysis is in progress starting from the GS constants obtained by Goroya et al. and with the support of electronic structure calculations.^d

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