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► To cite this version:

Pierre Asselin, Sathapana Chawananon, Manuel Goubet, Robert Georges, Anthony Roucou, et al.. High resolution Mid-Infrared spectroscopy of Volatile Organic Compounds from Fourier Transform and Quantum Cascade Laser measurements: case of 2-furfural. GDR NanoTeraMIR Meeting 2023, LPCA, Dunkerque, May 2023, Dunkerque (59140), France. hal-04295116

HAL Id: hal-04295116

<https://hal.science/hal-04295116>

Submitted on 20 Nov 2023

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High resolution Mid-Infrared spectroscopy of Volatile Organic Compounds from Fourier Transform and Quantum Cascade Laser measurements: case of 2-furfural

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As a reaction product of biomass combustion, the ortho-isomer 2-furfural (2-FF) is a primary pollutant in the atmosphere. Laboratory studies demonstrated that emission rates of 2-FF and other furan-like compounds as furan and methylfurans, measured during combustion ranged up to 120 times higher than CO, making them marker volatile organic compounds for fire warning system [1,2]. 2-FF disappears rapidly by atmospheric oxidation processes with OH and NO₃ during day and night times leading to the formation of secondary organic aerosols which affect the climate. Its contribution to the radiative forcing, still poorly known, fully justifies the interest to monitor 2-FF directly in the atmosphere or in atmospheric simulation chambers to characterize its ability to produce secondary organic aerosols [3,4].

The present study reports an extensive jet-cooled rovibrational study of *trans* and *cis* conformers of 2-FF in the mid-IR region using two complementary set-ups, a continuous supersonic jet coupled to a high resolution Fourier transform spectrometer on the IR beamline of the SOLEIL synchrotron (JET-AILES) [5] and a pulsed jet coupled to a mid-IR tunable quantum cascade laser spectrometer (SPIRALES).[6] In a first step, jet-cooled spectra recorded at rotational temperatures ranging between 20 and 50 K have been exploited to derive reliable excited state molecular parameters for a ten of vibrational bands of 2-FF in the fingerprint region (700-1750 cm⁻¹). These parameters allow reproducing the mid-IR spectra at any temperature and any instrumental resolution at the experimental accuracy. In the present case, they have been used to reconstruct the vibrational cross-sections referenced in the HITRAN atmospheric database measured at room temperature in a N₂ dilution. Such an approach evidenced the major contribution of hot bands in the room temperature mid-IR spectra of 2-FF, which represents about 50% of the fundamental bands. To go further in assigning the hot band pattern and improving the modeling of room temperature rovibrational cross-sections require imperatively using highly correlated *ab initio* methods to provide accurate anharmonic coefficients $\chi_{i,j}$ from a reliable anharmonic force field.

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