ROVIBRATIONAL SPECTROSCOPY OF TRANS- AND CIS-CONFORMERS OF 2-FURFURAL FROM HIGH RESOLUTION FOURIER TRANSFORM AND QCL INFRARED MEASUREMENTS

P. ASSELIN, S. CHAWANANON, Sorbonne Université, MONARIS, CNRS, UMR8233, 4 Pl Jussieu, F-75005 Paris, France; J. A. CLAUS, M. GOUBET, Univ. Lille, CNRS, UMR8523 - PhLAM - Physique des Lasers Atomes et Molécules, F-59000 Lille, France; A. ROUCOU, Université du Littoral Côte d’Opale, UR4493, LPCA, Laboratoire de Physico-Chimie de l’Atmosphère, F-59140 Dunkerque, France; R. GEORGES, Université de Rennes, CNRS, IPR (Institut de Physique de Rennes) - UMR 6251, F-35000 Rennes, France; J. SOBCZUK, Smoluchowski Institute of Physics, Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, Lojasiewicza 11, 30-348 Krakow; O. PIRALI, Université de Paris-Saclay, CNRS, Institut des Sciences Moléculaires d’Orsay, 91405 Orsay, France; C. BRACQUART, A. CUISSET, Université du Littoral Côte d’Opale, UR4493, LPCA, Laboratoire de Physico-Chimie de l’Atmosphère, F-59140 Dunkerque, France

The ortho-isomer 2-furfural (2-FF) is a primary atmospheric pollutant produced from biomass combustion which is also involved in oxidation processes leading to the formation of secondary organic aerosols. Its contribution to the radiative forcing, poorly known, fully justifies to monitor 2-FF directly in the atmosphere or in atmospheric simulation chambers to characterize its reactivity.

This study presents a jet-cooled rovibrational investigation of trans and cis conformers of 2-FF in the Mid-IR. Jet-cooled spectra were recorded at 20-50 K using two setups: a supersonic jet coupled to a high-resolution Fourier transform spectrometer (JET-AILES) and a pulsed jet coupled to a mid-IR tunable quantum cascade laser spectrometer (SPIRALES).

Reliable excited state molecular parameters for trans- and cis-2-FF vibrational bands were derived from fitting 11,376 and 3,355 lines distributed over 8 and 3 vibrational states (including the ground state) with a root-mean-square of 12 MHz, respectively. The middle resolution spectrum of 2-FF recorded at 298.15 K available in the HITRAN database was reconstructed by extrapolating the data derived from our low-temperature high-resolution analyses. The reconstruction provided cross-sections of each vibrational band for both trans- and cis-2-FF conformers in the 700-1800 cm\(^{-1}\) region. In addition, we demonstrated that incorporating hot bands, accounting for 40-63% of the fundamental band, in our simulation was crucial for accurately reproducing HITRAN vibrational cross-sections of 2-FF with a deviation under 10%.