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Session Categories (Keywords) by Relevance: Atmospheric science — Infrared/Raman — Large molecules
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Mini-Symposia Requested: None — None

Competing for Rao Prize? No

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JET-COOLED AND LONG PATH CELL HIGH RESOLUTION INFRARED SPECTROSCOPY OF FURFURAL CONFORMERS FROM FOURIER TRANSFORM AND QCL MEASUREMENTS

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Furfural, C_4H_3OCHO , is a volatile organic compound produced from biomass burning. Its oxidation may lead to secondary organic aerosol formation, making necessary to provide accurate spectroscopic data to evaluate its impact. Two conformations exist in the gas phase, with the oxygen atoms oriented in a more stable *trans* configuration than the *cis* one. Durig et al.^a exploited far-infrared (IR) data to determine relative stabilities and the conformational barrier height. Motiyenko et al.^b realized extensive microwave spectroscopic studies providing molecular parameters in the ground state (GS) and low-lying vibrational states up to 400 cm^{-1} . No splitting due to the internal rotation of the CHO top has been observed in these states. We report here a high resolution study of furfural on a wide infrared range combining the Jet-AILES set-up, a continuous supersonic jet on the IR AILES beamline at SOLEIL, and a long path cell, both coupled to a Fourier Transform Spectrometer and the SPIRALES set-up at MONARIS, a pulsed supersonic jet coupled to mid-IR quantum cascade lasers^c. In the fingerprint region, 7 bands of *trans*- and 2 bands of *cis*-furfural were recorded at low temperature. About 15000 lines from GS and 7(2) excited states (ES) of *trans*(*cis*-)furfural, respectively, were fitted within experimental accuracy. In the far-IR range, global fits including GS and ES rotational and ES rovibrational transitions enable to refine molecular parameters derived from the microwave study and to determine precise vibrational band centers.

^aT. S. Little, J. Qiu, J. R. Durig, *Spectrochimica Acta*, 45A, 789-794 (1989)

^bR. A. Motiyenko, E. A. Alekseev, S. F. Dyubko, F. J. Lovas, *J. Mol. Spectr.*, 240, 93-101 (2006), R. A. Motiyenko, E. A. Alekseev, S. F. Dyubko, *J. Mol. Spectr.*, 244, 9-12 (2007)

^cP. Asselin, J. Bruckhuisen, A. Roucou, M. Goubet, M-A. Martin-Drumel, A. Jabri, Y. Belkhdja, P. Souillard, R. Georges, A. Cuisset, *J. Chem. Phys.* 151, 194302 (2019), S. Chawananon, O. Pirali, M. Goubet, P. Asselin, *J. Chem. Phys.* 157, 064301 (2022)

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