

## MILLIMETER-WAVE SPECTROSCOPY OF METHYLFURAN ISOMERS: LOCAL vs GLOBAL TREATMENT OF THE INTERNAL ROTATION

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Methylfurans (MF) are methylated aromatic heterocyclic volatile organic compounds (VOCs) and primary or secondary pollutants in the atmosphere due to their capability to form atmospheric particles such as secondary organic aerosols (SOAs).<sup>1</sup> MFs are produced by cracking biomass such as wood combustion and the pyrolysis of biomass, lignin and cellulose.<sup>2</sup> Therefore there is a fundamental interest to monitor these molecules in the gas phase. The high resolution spectroscopic studies of methylated furan compounds, except 2-MF<sup>3</sup>, are generally limited to pure rotational spectroscopy in the ground state. This might be explained by the difficulties arisen from the internal rotation with a medium barrier and the complexity of the vibrationally excited state rotational spectra. As Finneran *et al.* for 2-MF, we faced the same difficulties for 3-MF to treat the first torsional state ( $\nu_t = 1$ ) using a local approach (XIAM<sup>4</sup>) and therefore the global treatment, including all torsional levels given by the BELGI code<sup>5</sup>, was used. This gave us access to the  $V_6$  term characterising the anharmonicity of the potential, together with some higher order perturbation and coupling terms. Carrying out a BELGI global fit of  $\nu_t = 0$  and  $\nu_t = 1$  states using our new assignment for 3-MF and the assigned transitions of Finneran *et al.* for 2-MF enabled us to compare the molecular parameters of these two isomers.

<sup>1</sup> X. Jiang, *Atmos. Chem. Phys.* **2019**, 19, 13591-13609.; <sup>2</sup> M. Perzon, *Biomass and Bioenergy*. **2010**, 34, 828-837.; <sup>3</sup> I.A. Finneran, *J. Mol. Spectrosc.* **2012**, 280, 27-33.; <sup>4</sup> H. Hartwig and H. Dreizler, *Z. Naturforsch.*, **1996** 51a, 923; <sup>5</sup> I. Kleiner, *J. Mol. Spectrosc.*, **2010**, 260(1), 1-18.