

## EXPLORING THE BINDING OF METHANOL WITH FURANS

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Recently, an infrared study on the complex of dimethylfuran and methanol showed only a slight preference for methanol to bind via an  $\text{OH} \cdots \text{O}$  hydrogen bond versus the  $\text{OH} \cdots \pi$  bond.<sup>a</sup> From this work, a ‘blind challenge’ was undertaken to compare the quantum chemical and experimental results of the microsolvation of a furan ring in methanol, with varying degrees of methyl substitution on furan, having a focus on methanol binding sites.<sup>b</sup> The hope of the challenge is to gauge how well experiment and theory can agree on site preference when the energy difference is near 1 kJ/mol, and ultimately to discern which theoretical models perform the best.

To this end, we present the rotational spectrum and structural analysis of the dimethylfuran complex with methanol. The rotational spectrum was recorded on the Hamburg COMPACT (compact-passage acquired coherence technique) microwave spectrometer from 2 – 18 GHz.<sup>c</sup> The observed spectrum is complicated by the internal rotation of three methyl tops, two from the dimethylfuran and one from the methanol. Each methyl top adds additional torsional angular momentum to the rotating complex, which subsequently splits the rotational energy levels yielding a complex set of torsion-rotation transitions. The resulting methyl top tunneling parameters are essential to aid in the structure determination of the complex. These results will be compared with the furan methanol results to see the effect of methylation on site preference.

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<sup>a</sup>A. Poblitzki et al, *Phys. Chem. Chem. Phys.* 2016, 18, 27265.

<sup>b</sup>H. C. Gottschalk et al, *J. Chem. Phys.* 2018, 148, 014301.

<sup>c</sup>D. Schmitz et al, *J. Mol. Spectrosc.* 2012, 280, 77.