# TOWARDS UNDERSTANDING THE SOLVENT-ROLE IN THE CATALYSIS OF THE BIOMASS-MOLECULE 6-AMYL-$\alpha$-PYRONE USING MICROWAVE SPECTROSCOPY

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6-amyl-$\alpha$-pyrone (6PP) is a biomass molecule that is widely used in the synthesis of industrial and pharmaceutical products. 6PP offers a green and sustainable route in the preparation of industrial chemicals such as linear ketones and hydrocarbon fuels. It is catalytically hydrogenated to produce $\delta$-decalactone (DDL). This reaction, carried out in different solvents under similar conditions, is reported to produce significant variation in DDL yield varying from 6% to 79%.[1] Such dramatic variations in yield during the reaction can be attributed to numerous reasons, such as the dielectric constant of solvents, or different kinds of solute-solvent interactions during the reaction.

In this work, we study the structure of 6PP and its solute-solvent interactions using chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy. This technique coupled with supersonic expansion reveals accurate structures of molecules and weakly bound complexes isolated in the gas phase. 6PP is highly flexible due to the presence of the pentyl chain. We first investigate the conformational flexibility in 6PP and then its complexes to understand the effect of the solvent molecule on the structure of 6PP. We choose two solvents, ethanol and cyclohexane one giving the best yield and the other one giving moderate results to study how the inter-molecular interactions affect the reaction yield. The observed structural changes in 6PP upon complexation, as well as the preferred intra- and intermolecular interactions, will be discussed.

[1] M. I. Alam, T. S. Khan, M. A. Haider, *ACS Sustainable Chemistry and Engineering* **2019**, *7*, *3*, 2894-2898.