CONFORMATIONAL LANDSCAPE AND INTERNAL DYNAMIC OF LEVULINIC ACID FROM BROADBAND ROTATIONAL SPECTROSCOPY

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Lignocellulose is the most abundantly available raw material on the Earth for the production of biofuels. [1] The main challenge is to produce useful chemicals from it. A variety of chemicals and biomolecules are produced via the hydrothermal conversion of waste biomass. Among the produced products is levulinic acid (LA). This biomolecule is considered to be of the top 10 chemical compounds, [2] as it has an important potential to be considered as a platform chemical. [3] It is used in the production of diverse chemical compounds in different area such as pharmaceuticals, herbicides, polymers, fuels etc. Gas phase rotational studies permit a better understanding of intermolecular interactions that control the conformation landscape of molecules and their internal dynamics. We present herein, a broadband rotational study in jet-cooled conditions, of the relevant levulinic acid in the 6-18 GHz range. [4] One conformer has been identified in the gas phase. The spectrum showed clearly that the lines were split. This splitting is due to the internal rotation of the methyl group. The A and E states lines were assigned and fitted, and the experimental barrier of the methyl torsion was determined.

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[2] T. Werpy and G. Petersen, Top Value Added Chemicals from Biomass: Volume I, Results of Screening for Potential Candidates from Sugars and Synthesis Gas. United States N. p.(2004)

[3] G.C. Hayes and C.R. Becer, Polymer Chemistry, **11**, 4068–4077 (2020)

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