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Microwave Spectroscopic Characterization of Furan–Formic Acid Clusters: Large-Amplitude Motions and Noncovalent Interaction Analysis

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Proton transfer (PT) reactions are essential in many chemical and biological systems due to their critical roles in energy conversion processes. Uncovering the mechanisms of PT is vital for controlling tunneling rates and advancing tunneling applications. The formic acid dimer undergoes double proton transfer; as a result, it serves as a well-established prototype for studying tunneling mechanisms. Herein, we measured the rotational spectrum of the formic acid-furan system and identified the Furan$-$FA$_n$ clusters with $n = 2 - 4$. The results reveal that in the Furan$-$FA$_2$ cluster, the tunneling dynamics become more intricate. Specifically, two large-amplitude motions are involved: the rotation of the furan molecule coupled with the double proton transfer within the formic acid dimer. For the larger clusters, Furan$-$FA$_3$ and Furan$-$FA$_4$, no distinct splitting patterns are observed under the resolution of the broadband microwave spectrum (approximately 15 kHz). However, the two structures differ significantly, exhibiting notable changes in the noncovalent interactions both among the formic acid molecules and between formic acid and furan. Therefore, we performed many-body energy decomposition (MBE) and noncovalent interaction (NCI) analyses to investigate the competition among different types of noncovalent interactions present in these species.

Keywords

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