Conformational Panorama of a Chiral Carboxylic Acid and its Aggregates in a Supersonic Jet Expansion, a Cold Rare Gas Matrix and Solution

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A molecule is chiral if its mirror image cannot be superimposed onto itself. When a chiral molecule interacts with another chiral entity, such as another chiral molecular target or chiral light, it can recognize the chirality of the target or generate a chiroptical response, respectively. In this presentation, I will first discuss conformational panorama of tetrahydro-2-furoic acid (THFA), a chiral carboxylic acid, and chirality recognition in its binary dimer.[1] By using broadband chirped pulse Fourier transform microwave spectroscopy, aided by CREST,[2] a semiempirical quantum chemistry conformational search tool, and DFT calculations, we examined the preferred conformations landscape of the binary THFA adducts in detail. The subsequent matrix isolation vibrational circular dichroism study reveals a much different conformational distribution of the binary adducts.[3] Further experiments of THFA in aqueous solution demonstrate new preferred binary species.[4] We emphasize the connection between the gas phase results obtained using high resolution rotational spectroscopy with those obtained in the condense phases. The unusual conformational distributions and chirality controlled conformational preferences under different conditions will be discussed.

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References

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