

Conformational diversity of carboxylic acids

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Small α -dicarbonyl compounds are abundant pollutants in the atmosphere. They exist as gas-phase molecular clusters; they also form solid or liquid particles thus contributing to the formation of secondary organic aerosols. The latter have a strong impact on the climate and on human health.

The conformational landscape of α -dicarbonyl compounds is very complex because of their multiphasic chemistry. Indeed, not only does environment affect their chemical reactivity but also their preferential geometry. Precise knowledge of the structure in these different environments is crucial since the aggregation properties of small pollutants can be steered by the structure.¹

Here we present the vibrational spectrum of succinic acid, a small dicarboxylic acid abundantly found in Antarctica, in KBr pellet and argon cryogenic matrix. Aided by an extended theoretical study, the IR signatures are discussed to shed light on the factors responsible for the stabilizing interactions in succinic acid.²

¹ Pollet, R.; Chin, W. Reversible Hydration of α -Dicarbonyl Compounds from Ab Initio Metadynamics Simulations: Comparison between Pyruvic and Glyoxylic Acids in Aqueous Solutions. *J. Phys. Chem. B* **2021**, *125*, 2942. –2951 *J. Chem. Phys.* **2012**, *137*, 194313.

² Da Silva Sa, L.; Camiruaga, A. et al. Unveiling the conformational diversity of succinic acid: Insights from IR spectroscopy and quantum chemical calculations. *Low Temp. Phys.* **2024**, submitted.