Structure-Energetics Relationships in Organic Molecular Solids

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The ability to plan and control the assembly of organic molecules in crystals to produce materials tailored for an application is a topic of considerable current interest.

In this context, the study of families of structurally related compounds is important to provide clues on how systematic changes in a molecular framework can influence the crystalline structure and the lattice energetics. This will be illustrated through recent studies from our laboratory focused on fumaric acid, alkyl fumarates, and co-crystals thereof, that relied on structural determinations by X-ray diffraction and thermodynamic measurements (e.g. solution and sublimation calorimetry, solubility).

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