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Systematic studies of polymorphism in structurally related compounds: the 4-hydroxybenzoyl family

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Polymorphism, the ability of a molecule to crystallize in multiple solid forms, is commonly observed in many organic compounds. Although the molecule remains the same, packing differences can lead to significant variations in the physicochemical properties (e.g., color, melting point, solubility) of the material. This represents a major concern for various chemical industries (e,g. dyes, agrochemicals, or pharmaceuticals), which rely on the production of materials with highly reproducible properties.

Insights into how the complex interplay of structural, thermodynamic, and kinetic factors influences the formation of different crystal structures at a molecular level, can be obtained by the systematic analysis of polymorphism in families of structurally related molecules. An attractive target for this type of studies is the 4-hydroxybenzoyl family of compounds, with the general formula $HOC_6H_4C(O)R$ (R = H, alkyl), where the molecules differ only in the length of the alkyl chain substituent. These compounds are prone to polymorphic behavior [1-3], displaying examples of both conformational and non-conformational polymorphism, similar and dissimilar polymorphic structures, as well as monotropic and enantiotropic relationships.

This work presents a general overview of our studies on this family of compounds, with a focus on the illustration of how to identify and study different types of polymorphism and show how seemingly small molecular modifications can result in a variety of structural organizations.

Figure 1. HOC_6H_4COR compounds studied in this work.

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