Packing Energetics in 4-HOC_6H_4COR Compounds: The Influence of the Side Chain

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Assessing how systematic changes in molecular structure influence the packing of a crystalline solid, and its physical properties, is a fundamental issue for the understanding of crystallization phenomena. Such studies can offer insights into the design and synthesis of molecular solid-state structures, with specific properties, through the control of their intermolecular interactions. This is of considerable technological interest, as different packing architectures can strongly affect the manufacture and processing of a product and its end use characteristics (e.g., the color of dyes, the conductivity organic conductors, or the bioavailability of drugs).

Compounds with the 4-HOC_6H_4COR backbone, containing H-bond donor (−OH) and acceptor (−C(O)R) substituents separated by a phenyl ring, are well suited for this type of studies since they have been shown to be susceptible to polymorphism, as found, for example, in the cases of HBA, HAP, and HVP (Figure 1),[1-3] and can provide information on how the length of the R side chain impacts on the observed crystallization patterns and crystal structures.

In this work the thermodynamic properties (e.g. enthalpies of fusion and sublimation) of different 4-HOC_6H_4COR compounds (Figure 1), and their dependence on the packing architectures, were analyzed as a function of the length of the side chain.

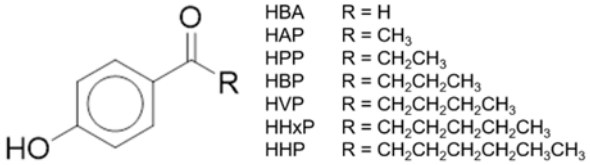

Figure 1. 4-HOC_6H_4COR compounds studied in this work

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