P063 Screening Polymorphism in 4-HOC₆H₄COR Compounds

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Polymorphism, the ability of a molecule to crystallize in more than one solid structure, is a phenomenon commonly observed in many organic compounds. Different packing arrangements are often accompanied by changes in the physical and chemical properties of the solid (e.g. color, melting point, solubility, etc.), and this represents a major challenge for the industrial production of organic materials with highly reproducible properties. Systematic studies of polymorphism using families of organic crystals where the different building blocks are structurally related molecules are particularly interesting to understand how the interplay of molecular size, shape and types of interaction may affect the packing architecture and the relative stability of crystal forms. One such family is the one with 4-HOC₆H₄COR backbone, that has H-bond donor (OH) and acceptor (C(O)R) substituents separated by a phenyl ring, since they have been shown to be prone to polymorphism, both due to changes in their molecular conformation (such in the case of HAP) [1] or through adjustments in their packing architecture (as in HBA and HVP), [2, 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-HOC6H4COR compounds (Figure 1), and their dependence on the packing architectures, were analyzed as a function of the length of the side chain.

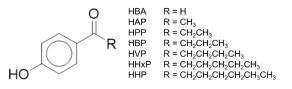


Figure 1: 4-HOC₆H₄COR compounds studied in this work

References

[1] Bernardes, C. E. S.; Piedade, M. F. M.; Minas da Piedade, M. E. Cryst. Growth Des. 2008, 8, 2419-2430.

[2] Lopes, C. S. D.; Bernardes, C. E. S.; Piedade, M. F. M.; Diogo, H. P.; Minas da Piedade, M. E. Eur. Phys. J. Sp. Top. 2017, 226, 849-855.

[3] Simões, R. G.; Bernardes, C. E. S.; Minas da Piedade, M. E. Cryst. Growth Des. 2013, 13, 2803-2814.

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