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Polymorphism in Organic Compounds:4'-Hydroxyvalerophenone, a Case of Conformational Polymorphism

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Polymorphism, the ability of a molecule to crystallize in more than one solid structure, is commonly observed in many organic compounds. Because different packing arrangements are often accompanied by changes in the properties of the solid (e.g. color, melting point, solubility) this represents a challenge for the industrial production of organic materials with highly reproducible properties. The systematic analysis of polymorphism in families of structurally related molecules can offer insights into how the interplay of molecular size, shape, and intermolecular interactions influences the packing architectures and relative stability of different crystal forms. 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. Polymorphism was previously identified in various $HOC_6H_4C(O)R$ compounds, both due to changes in the molecular conformation (e.g. 4'-hydroxyacetophenone) [1] or through adjustments in the packing architecture (e.g. 4-hydroxybenzaldehyde) [2].

In this work, the polymorphic behaviour of 4'-hydroxyvalerophenone (HVP, $C_{11}H_{14}O_2$, Figure 1), is analysed from structural and energetic perspectives. From the obtained results, the occurrence of conformational polymorphism in HVP, when recrystallizing the compound from the melt (Form II), was confirmed, and the thermodynamic relationship between the two forms was determined.

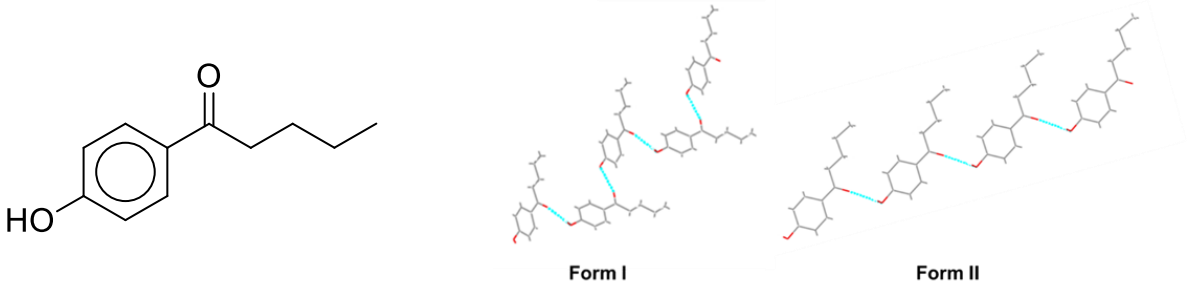

Figure 1. Molecular structure of 4'-hydroxyvalerophenone (HVP) and crystal structure of both polymorphs.

Acknowledgements

Support for this work was provided by FCT through projects PTDC/QUI-OUT/28401/2017 (LISBOA-01-0145-FEDER-028401) and UID/MULTI/00612/2013. R. G. Simões, C. E. S. Bernardes and C. S. D. Lopes acknowledge financial support from the grants SFRH/BPD/118771/2016, SFRH/BPD/101505/2014, and SFRH/BD/128794/2017, respectively.The authors also acknowledge the COST Action CM1402.

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