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Experimental and Theoretical Study of Low Temperature Solid-Solid Phase Transition in 4'-Hydroxyacetophenone Polymorphs

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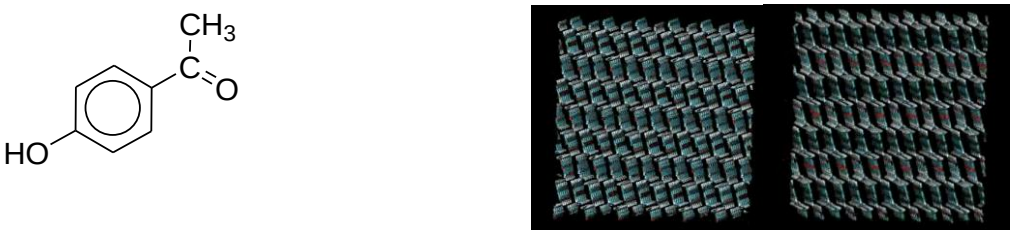
Polymorphism, the ability of a substance to crystallize in more than one lattice arrangement, is currently a major concern for the manufacture of organic products, since each crystal form can exhibit significant differences in physicochemical properties (e.g. fusion temperature, solubility/dissolution rate). For this reason, each polymorph corresponds, in fact, to a different material. To control polymorphism it is extremely important to understand the stability relationships between different polymorphs under specific pressure-temperature conditions, so that transitions to unwanted phases can be prevented during production and storage of polymorphic materials.

4'-Hydroxyacetophenone (HAP; Figure 1a) is a compound with significant commercial applications and additional potential end uses. Two polymorphs of HAP have been reported up to now, which are related by an enantiotropic solid-solid phase transition that occurs at ~303 K.[1,2] Recent adiabatic calorimetry and neutron diffraction studies revealed a new phase transition in both polymorphs at ~79 K, which, according to the structural results, does not involve a modification in the crystal packing of the two polymorphs.[3] In this work, molecular dynamics simulations were used to investigate the nature of this transition. The obtained results suggest that the observed changes are related with an order-disorder transition, and the existence of a modulation effect below 79 K (Figure 1b).



(a) (b)

Figure 1. (a) 4'-Hydroxyacetophenone (HAP); (b) Molecular dynamic snapshots, showing a modulation effect on the crystal structure of HAP form I at 10 K.

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