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The Effect of Tailor-made Additives on Crystal Growth of Methyl paraben: Experiments and Modelling

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ABSTRACT

In this study, methyl paraben (MP) was selected as the model component, and acetaminophen (APAP), p-methyl acetanilide (PMAA) and acetanilide (ACET), which share the similar molecular structure as MP, were selected as the three tailor-made additives to study the effect of tailor-made additives on the crystal growth of MP. HPLC results indicated that the MP crystals induced by the three additives contained MP only. Photographs of the single crystals prepared indicated that the morphology of the MP crystals was greatly changed by the additives, but PXRD and single crystal diffraction results illustrated that the MP crystals were the same polymorph only with different crystal habits, and no new crystal form was found compared with other references. To investigate the effect of the additives on the crystal growth, the interaction between additives and facets was discussed in detail using the DFT methods and MD simulations. The results showed that APAP, PMAA and ACET would be selectively adsorbed on the growth surfaces of the crystal facets, which induced the change in MP crystal habits.

Keywords: A1. Adsorption; A1. Computer simulation; A1. Impurities; A1. Single crystal growth; B1. Aromatic compounds

1. Introduction