Solvent Influence on Morphology of OH-1 Crystal by Molecular Modelling Study

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Crystal morphology is one of the important factors in crystallization process design and solvents have an influence on crystal growth habit. In this work, molecular modelling was carried out to predict solvent effect on crystal morphology of OH-1(2-(3-hydroxystyryl)-5,5-dimethylcylcohex-2-enylidene) malonontirile). Surfaces possible to appear were generated using the intrinsic crystal structure of OH-1 reported in Kwon's experimetnal work. Interaction of solvents and crystal surfaces was examined by performing molecular dynamics (MD) simulation and geometry optimization. Attachment energies of crystal on each surface were calculated considering interaction energies of solvents. Crystal morphologies were changed in the presence of solvents from pure morphology of OH-1. Organic polar solvents affected on interaction of crystal molecule with crystal surface by having a stable interaction on polar surfaces and this resulted in growth rates of crystal surfaces.