Prediction for Solvent Effect on Crystal Morphology of an Energetic Material by a Molecular Modeling Technique

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Final performance of high energy density explosives depends on shape, particle size and packing density of molecular explosives. Those factors may be modified by control of nucleation and crystal growth conditions such as crystallization methods, solvents, additives, etc.. In the present study, a cooling method was used for the observation of morphological change of ADNBF (7-amino-4, 6-dinitrobenzofuroxan) crystals with various solvents. Crystal surface properties and interactions between ADNBF molecule on crystal surfaces and each solvent were investigated and interpreted by the molecular modeling software Materials Studio 4.0.