

Effects of seeding-method on Polymorphs of HNIW in Drowning-out Crystallization

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To crystallize selectively forms β and ϵ of Hexanitrohexaazaisowurtzitane (HNIW), nucleation behavior and supersaturation level were studied in mixture solvents such as ACT/IPA, ACN/IPA, DMSO/IPA and EA/IPA. The effect of supersaturation on induction time and nucleation rate was evaluated by comparison between nucleation mechanisms of seeded and unseeded crystallizations. Experimental results indicate that the polymorph obtained by crystallization depends on the type of seed crystals, amount of seed crystals, and seeding point. Heterogeneous nucleation was desirable for the formation of ϵ -form. The β -form corresponds to primary nucleation, i.e., homogeneous and heterogeneous nucleations. The contribution of supersaturation to crystallization of the two crystalline forms of HNIW was investigated. The theoretical relationship between maximum supersaturation and induction time was verified to determine the nucleation behavior of the polymorphic forms for seeded and unseeded crystallizations.