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The path to achieving molecular dispersion in an extremely dense reactive mixture JIGNESHKUMAR PATEL, ZOU XIANG, SHAW HSU, University of Massachusetts Amherst, ANDREW SCHOCH, Saint-Gobain Research & Development — In any multicomponent reactive system, a uniform and continuous dispersion of reactants is necessary to achieve a complete reaction. In this study, we have examined the role of one additional component to disperse two seemingly unlikely reactants, including a highly crystalline hexamethylenetetramine (hexa) and strongly hydrogen bonded phenol formaldehyde resin. By combining information from NMR, infrared spectroscopy and differential scanning calorimetry, we were able to decipher the role of specific intermolecular interactions in order for this additional component to dissolve the highly crystalline hexa and to plasticize the phenol formaldehyde resin in this crosslinking reaction. It is clear that the presence of the third component increased the segmental mobility, disrupted the hydrogen bonded matrix, and freed the hydroxyl units, which further increased the solubility of hexa. Both the endothermic and exothermic transitions are accounted for in the calorimetric data obtained. For the first time, it is possible to understand the miscibility behavior of this multicomponent system. By designing the additional component to form a hydrogen bond with one or more N of the highly symmetric hexamethylenetetramine, it is then possible to obtain the effective molar ratio of each component needed to complete the crosslinking reaction efficiently. The understanding of this system is applicable to a broad range of reactive systems.

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