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Investigating dynamic phase behaviors in molecular hydrates

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A large fraction of organic molecules can crystallize as hydrates, including all four of the DNA nucleobases. Hydrated (H) and anhydrous (A) phases exhibit different physical properties. Here we examine the properties of thymine hydrate (TH) and isomorphous solid solutions of TH prepared with 5-aminouracil (AUr). Using neutron backscattering spectroscopy (NIST Center for Neutron Research) and thermal analysis methods, we are able to observe and quantify significant differences in the local environment of diffusive water and the thermal stability of these hydrate phases. Complementary time-resolved synchrotron PXRD studies (Advanced Photon Source, 17-BM) make it possible to monitor both subtle and dramatic structural changes that occur during the solid state dehydration processes under controlled environmental conditions. This work serves to illustrate how the reaction kinetics and dehydrated products can be rationally tuned by altering the chemical purity of the precursor hydrate phase.