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**Studies of Phase Relationships in Cocrystal Systems.** Raymond E. Davis, Keith A. Lorimer, Matthew A. Wilkowski, Jr., Joseph H. Rivers, Dept. of Chemistry & Biochemistry, Univ. of Texas at Austin, Austin, TX 78712; Kraig A. Wheeler, Jeffrey Bowers, Dept. of Chemistry, Delaware State Univ., Dover, DE 19901.

We are using several methods to investigate phase relationships and comparative structures of cocrystalline systems. Video-assisted thermomicroscopic analysis can give a rapid visual display of the melting point phase diagram. Various single/mixed phase possibilities – conglomerate crystallization with a single eutectic, formation of one or more stoichiometric cocrystalline phases with two or more eutectics, or solid solution formation – can be readily examined and distinguished by this technique. Standard thermal methods such as differential scanning calorimetry provide data for experimental determination of the melting point phase diagram. We have also investigated the simulation of these phase diagrams from a combination of experimental thermal data and the Schröder-Van Laar and Prigogine-DeFay equations. Powder X-ray diffraction data provide an additional means of studies of single vs. mixed phases. Finally, single crystal structure determinations allow full structural characterization of individual components and cocrystals.

Results obtained by such methods will be illustrated for various systems, including some enantiomer/racemate/quasiracemate systems whose structures we have reported previously and some other hydrogen-bonded cocrystals.

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