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Crystal Engineering, Co-crystals and Polymorphs. J. Bernstein, Dept. of Chemistry, Ben-Gurion Univ. of the Negev, Beer-Sheva, 84105, Israel.

Crystal engineering involves the design and preparation of crystal structures by taking advantage of specific intermolecular interactions. The building blocks of the crystal structure are often referred to as supramolecular synthons. In many cases they are composed of a number of molecules which interact through hydrogen bonding that may be defined by the graph set of the hydrogen bonding pattern(s) involved in the specific interactions. One of the most common of the hydrogen bonding patterns utilized in crystal engineering has been the R2,2(8) pattern. We have recently been investigating the possibility of utilizing the R4,2(8) pattern for crystal engineering, since it has the potential for generating cocrystals composed of up to four components. In the course of carrying out experiments to generate crystal structures containing the R4,2(8) hydrogen bonding motif, we have obtained a number of new polymorphs of at least one of the components of the intended cocrystal. Although the desired and designed crystal structure was not obtained, the fact that new polymorphs were obtained suggests that the second component serves as either an inhibitor of some crystal forms and/or a promoter of other crystal forms. Understanding these phenomena could lead to methods of designing or preventing new polymorphic structures or cocrystals.