

W0047

Hydrogen Bonding, Graph Sets, Cocrystals and Crystal Design. Joel Bernstein, Dept. of Chemistry, Ben-Gurion Univ. of the Negev, P.O. Box 653, Beer Sheva, 84105 ISRAEL.

Ken Trueblood's considerable scientific legacy stems from the fact that he was first and foremost a chemist, a quintessential practitioner, researcher and teacher of structural chemistry and chemical crystallography. He viewed a crystal structure as the source of chemical information on the molecular entity under study and the crystal structure associated with it.

Some of that legacy is manifest in current efforts to utilize specific intermolecular interactions, in particular hydrogen bonds, to facilitate the design and "construction" of crystals with varying degrees of essentially predetermined structure. Hydrogen bond patterns are readily characterized by the graph set designators, which aids in classifying and utilizing recognized patterns as potential building blocks for crystal design and construction. Such patterns may be homomolecular or heteromolecular, in the latter case providing a means for generating designed cocrystals, for instance for the modification of the structure and properties of pharmaceutically active materials.

In this talk we will review the use of graph sets in characterizing hydrogen bond patterns and their utilization in the design and preparation of cocrystals with at least two components.