



Book review

MAKING CRYSTALS BY DESIGN Methods, Techniques and Applications

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The book is written by a consortium of scientists from Germany, Israel, Italy, Japan, Spain, UK, USA and answer to the demand for books in the field of crystal engineering that has reached a new level of maturity. The work has an unconventional structure, in accordance, with this modern discipline-crystal engineering, which care be considered to be at the intersection of supramolecular and materials chemistry. It is an excellent handbook which covers and evaluates various and complex aspects of modern crystal engineering. The engineering of crystals targets the construction of their properties from *the convolution of the physico-chemical properties and intermolecular branding capacity of the bridling blocks with the periodicity and symmetry of the crystal*.

The book is structured into three parts which mainly refer to: geometry and design and reactivity, characterization and applications.

The first part, **GEOMETRY AND ENERGETICS** includes three chapters, written by different authors.

Supramolecular Interactions: Energetic Considerations (the first part, author: Angelo Gavezzoti) is a quite comprehensive work about the principles of the quantitative energetic evolution of intermolecular interactions, the basis of nonreactive chemical phenomena occurring among organic molecules in condensed phases. It discusses the problems of supramolecular intermolecular interaction considering enthalpy, entropy, free energy, giving also tutorial examples on dimerization energies, calculation of lattice energies, analysis of crystal structures.

The second chapter, *Understanding the Nature of the Intermolecular Interactions in Molecular Crystals. A Theoretical Perspective* (authors: Juan J. Novoa, Emiliana D'Oria and Maria A. Carvajal) offers a qualitative description of the

properties of the most relevant intermolecular interactions considering the packing of molecular crystals. Information about intermolecular interactions is obtained from theoretical considerations, together with statistical analyses of crystal packing. The basic principles of the nature, strength and directionality of the intermolecular interactions found in molecular crystals are highlighted. In this chapter the nature of single type of intermolecular interactions was analyzed, using sample systems such as gas-phase dimers, where is no competition among different interactions, completed by an analysis of the changes which occur when more than one intermolecular interactions is present in the systems.

The third chapter, *Networks, Topologies and Entanglements* (authors: Lucia Carlucci, Gianfranco Ciani and Davide M. Prasepia) describes some aspects regarding the rationalization of some supramolecular systems proceeding in order of increasing complexity, starting with the simplification of crystal structure in order to carry out a topological analysis of the individual idealized crystalline networks. Various types of entanglements of single motifs, including interpenetrated, polycatenated, and other networked arrays were considered and classified.

The second part, **DESIGN AND REACTIVITY** contains five chapters.

The first chapter, *Prediction of Reactivity in Solid-state Chemistry* (author Gerd Kaupp) introduced the topochemical principle on the basis of α - and β - cinnamic acid. The single-crystal-to-single-crystal reactions without crystal disintegrations are scrutinized that appears to only be possible if the shape of the product molecules did not significantly deviate from the starting molecules in the crystal. A comprehensive classification of the different shapes

and qualities of crystallographic cleavage planes and chapels is provided in order to demonstrate the predictive power of the experimental mechanism approach.

The second chapter, *Making Crystals by Reacting Crystals* (author Fumio Toda) discusses about reactions proceeding in the solid state, with very high concentration and selectivity. In addition, the solid state reactions have the advantages of reduced pollution, low costs, simplicity in process and handling. The occurrence of efficient solid-state reactions shows that the molecules reacting are able to move freely in the solid state. Host-guest inclusions complexation can occur by simply mixing and grinding both crystals in the solid state. Inclusion of crystals proceeds efficiently and stereoselectively to give one stereoisomer in a pure state. In some cases, an optically active product results from mixing and grinding host and guest crystals in the solid state. Selective inclusions complexation by contact of the racemic host crystal with ether vapor in the solid state can be controlled by adding a seed crystal.

The third chapter of the second part, *Making Crystals by Reactions in Crystals. Supramolecular Approaches to Crystal-to-Crystal Transformations within Molecular Co-Crystals* (authors: Tomislav Frišćić and Leonard R. MacGillivray) analyses the reliable methods to control molecular arrangements suitable for reactivity in the solid state derived from the principles of supramolecular chemistry. It also illustrates how the design of reactive multi-component solids or co-crystals can be achieved by exploiting non-covalent forces and the process of self assembly. Some examples were given, in order to provide insights into the benefits of co-crystals to both synthetic organic chemists and solid-state materials scientists. Also it is shown how intermolecular bound-forming reactions that generated crystalline products from crystalline reactants appeal to both areas.

The fourth chapter, *Making Coordination Frameworks* (author: Neil R. Champness) attempts to address some of the issues that need to be considered when preparing coordination frameworks. Also, it provides a guide for those coming into the area and also materials for thought to those who are established practitioners in the field. The process of coordination framework synthesis from initial design, through choice of the components of the desired framework is discussed, together with the choice of experimental conditions, considerations with respect to structural analysis and the ultimate understanding of framework structure and description.

The fifth chapter, *Assembly of Molecular Solids via Non-covalent Interactions* (authors: Christer B. Aakeröy and Nate Schultheiss) investigates two subject areas. First, it deals with an overview of strategies for the directed assembly of homomeric O-D, 1-D, 2-D and 3-D molecular architectures with specific, pre-determined and desirable connectivities and metrics is offered. Second a description of some design principles that have been devised and tested for the assembly of co-crystals, heterometric molecular solids, is given.

The third part of the book, **CHARACTERIZATIONS AND APPLICATIONS** includes four chapters.

The first chapter, *Diffraction Studies in Crystal Engineering* (authors: Guillermo Mingnez Espallargas and Lee Grammer) provides details about the manner the information in crystallography could be applied based on diffraction studies (diffraction of X-rays and neutrons by single crystals and polycrystalline powders). Some illustrative examples of diffraction experiments that move beyond structure determination from single crystal diffraction are given. Also, diffraction studies at different temperatures and pressures are examined, as well as charge density, all of them regarded as valuable inputs into crystals engineering development.

The second chapter, *Solid State NMR*, (author: Roberto Gobetto) gives information about solid state NMR and presents some recent results where the development of new pulse sequences have brought some insights into various aspects of the characterization of solid state materials. Solid state NMR is treated as a well established tool for molecular structure determination and particularly attractive in solid systems lacking order or homogeneity for crystallographic examination.

The third chapter, *Crystal Polymorphism: Challenges at the Crossroads of Science and Technology* (author Dario Braga and Joel Bernstein) give an introductory view of the phenomena of multiple crystal forms in general and polymorphism in particular. Also, some aspects on the scientific, commercial and ethical importance and implications of these phenomena are look at.

The fourth chapter of the third part, *Nanoporosity Gas Storage, Gas Sensing* (author Satoshi Takamizawa) focuses on new aspects of nanoporosity. It is emphasized that the crystalline material consisting of an organic frame is flexible, with a potential degree of freedom, even in its crystalline state. A weak physical adsorption interaction can lead to a change in the solid structure and can stabilize various gas adsorption states. It was demonstrated that the gas adsorption behavior of single – crystal adsorbents is related to whether they have crystal phases that can change depending on the amount and type of guest molecules and on the process of guest inclusion, via control of the host structural flexibility. The properties of crystal adsorbents, such as: homogeneity, anisotropy, integrity, transparency, with precise molecular design contributes to the advancement of new technique for future studies.

This book is an essential source of high quality information for the scientists working in this interdisciplinary field (chemists, materials scientist in the field of nanotechnology and pharmaceutical industry), analysts.

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