INTERACTION AND RECOGNITION IN MOLECULAR CRYSTALS

Molecular crystals are ideal models for the study of molecular interaction forces that are responsible for the different aggregation states of matter and which are important for supramolecular recognition processes relevant in chemistry, material science and biochemistry of the drug-receptor and enzyme-substrate interactions. The study of crystal packing within extended series of crystals (either designed ad hoc or derived from systematic investigation of crystallographic databases, also possibly integrated with thermodynamic and spectroscopic data as well as computational calculations) allows for the identification of intermolecular recognition forces that enable molecule to be part of stable aggregated species. The data analysis is performed with LFER (linear free-energy relationships) and structural correlation methods aimed at the definition of the reaction pathways and the identification of structure/properties relationships.

GOALS

(a) Systematic study of hydrogen bonding, its classification in chemical classes and formulation of general models capable of predicting the properties, with particular regard to structure and energetic. (b) Application of strong hydrogen bonding in chemistry, biochemistry, and material science. (c) Systematic study of charge transfer interactions in molecular crystals. Their importance in the determination of the crystal packing and in the definition of a general theoretical basis for molecular interactions. (d) Application of the understanding of the molecular interactions towards crystal engineering, with particular regard towards functional materials and co-crystals of pharmaceutical interest.

INSTRUMENTS AND METHODS

Systematic use of crustallographic and theromdynamic databases. Simulation of model molecules by quantum chemistry with either “ab initio” or DFT methods. Preparations of molecular crystals and co-crystals for the study of molecular interactions and their structural determination by X-ray diffraction technique at both room and cryogenic temperature.

MAIN SUBJECTS

Structural chemistry, Physical chemistry, General chemistry

RESEARCH GROUP

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