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Nota di contenuto	Organic Crystal Engineering; Contents; List of Contributors; Preface; 1. The Role of the Cambridge Structural Database in Crystal Engineering; 1.1 Introduction; 1.2 Organisation and Management of Crystallographic Information; 1.2.1 Validation of New Crystal Structures: Mogul; 1.2.2 Validation of Structural Discoveries: What is New and What is Not?; 1.3 Organisation of Crystallographic Information for Crystal Engineering; 1.3.1 IsoStar; 1.3.2 CSDContact; 1.3.3 CSDSymmetry; 1.4 New Tools for Database Research; 1.4.1 A General Tool for 3-D Searches of the CSD: 3DSEARCH; 1.4.2 Ad hoc Software 1.5 Search for Functional Group Exchanges: GRX1.6 Search for Solvated and Unsolvated Structures: Solvates; 1.6.1 Tools to Examine Structural

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2.2 Methods used to Predict Crystal Structures2.2.1 Search Methods; 2.2.2 Evaluating the Computer-generated Crystal Structures; 2.3 Current Capabilities of Crystal Structure Prediction; 2.3.1 The Blind Tests; 2.3.2 Further Assessments of Crystal Structure Prediction; 2.3.3 Flexible Molecules; 2.4 Exploration of Crystal Forms. A Case Study: Carbamazepine; 2.4.1 Polymorphism and the Influence of Small Molecular Changes on Packing; 2.4.2 Solvate and Co-crystal Formation; 2.4.3 Computational Solid Form Screening?; 2.5 Summary; Acknowledgements; References
3. Multi-component Pharmaceutical Crystalline Phases: Engineering for Performance3.1 Introduction; 3.2 Exploring Crystal Form Diversity; 3.3 High-throughput Experimentation; 3.4 Examples of 'Form and Formulation'; 3.4.1 Indinavir sulfate ethanolate - a case of a salt hydrate/solvate; 3.4.2 Norfloxacin - polymorphs, solvates, salts, complexes and co-crystals; 3.5 AMG517 and Celecoxib - 'Spring and Parachute' Approach; 3.5.1 -Lactam antibiotics and hydrates - the importance of crystallinity; 3.6 Carbamazepine - Stabilization Against a Hydrate
3.7 Theophylline:Phenobarbital - Two is Better Than One3.8 Delaviridine Mesylate - Material Misbehaviour; 3.9 Summary and Outlook; References; 4. Complex Formation of Surfactants with Aromatic Compounds and their Pharmaceutical Applications; 4.1 Introduction; 4.2 Structures of the Complexes Formed Between Surfactants and Aromatic Compounds; 4.2.1 Crystal structure of I (CTAB-p-hydroxybenzoic acid); 4.2.2 Crystal structure of II (CTAB-m-cyanophenol); 4.2.3 Crystal structure of III (CTAB-p-cresol); 4.2.4 Crystal structure of IV (CTAB-hydroquinone)
4.2.5 Crystal structure of V (CTAB-o-iodophenol)

Sommario/riassunto

Organic Crystal Engineering provides reviews of topics in organic crystal engineering that will be of interest to all researchers in molecular solid-state chemistry. Specialist reviews written by internationally recognized researchers, drawn from both academia and industry, cover topics including crystal structure prediction features, polymorphism, reactions in the solid-state, designing new arrays and delineating prominent intermolecular forces for important organic molecules.