

1. Record Nr.	UNINA9910826322103321
Titolo	The importance of Pi-interactions in crystal engineering : frontiers in crystal engineering // edited by Edward R.T. Tiekink, Julio Zukerman-Schpector
Pubbl/distr/stampa	Hoboken, NJ, : Wiley, 2012
ISBN	9786613621351 9781119940920 1119940923 9781280591525 1280591528 9781119945888 1119945887 9781119945895 1119945895
Edizione	[2nd ed.]
Descrizione fisica	1 online resource (402 p.)
Altri autori (Persone)	TiekinkEdward R. T Zukerman-SchpectorJulio
Disciplina	548/.3
Soggetti	Molecular crystals Supramolecular organometallic chemistry Crystal growth
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	The Importance of Pi-Interactions in Crystal Engineering; Contents; Preface; List of Contributors; 1 The CH/p Hydrogen Bond: Implication in Crystal Engineering; 1.1 Introduction; 1.1.1 Evidence and the Nature of the CH/p Hydrogen Bond; 1.1.2 Directionality of the CH/p Hydrogen Bond; 1.2 Cooperative Effect of the CH/p Hydrogen Bond; 1.2.1 Cooperative Effect as Evidenced by High-Level Ab Initio MO Calculations; 1.2.2 Cooperative Effect as Evidenced by Periodic Ab Initio MO Calculations; 1.2.3 Cooperative Effect as Evidenced by Stabilisation of Materials in Aromatic Nanochannels 1.2.4 Optical Resolution 1.3 CH/p Hydrogen Bonds in Supramolecular

Chemistry; 1.3.1 Crystal Packing; 1.3.2 Lattice Inclusion Type Clathrates; 1.3.3 Cavity Inclusion Type Clathrates; 1.4 Crystallographic Database Analyses; 1.4.1 CH/p Hydrogen Bonds as Evidenced by CSD Analyses; 1.4.2 Systematic CSD Analyses; 1.5 Systematic CSD Analyses of the CH/p Hydrogen Bond; 1.5.1 Method and General Survey of Organic Molecules; 1.5.2 Organometallic Compounds; 1.6 Summary and Outlook; Acknowledgments; References; 2 New Aspects of Aromatic p . . . p and C-H . . . p Interactions in Crystal Engineering 2.1 Introduction 2.1.1 Planar Aromatic Molecules; 2.1.2 Edge-Face (EF) and Offset Face-Face (OFF) Interactions; 2.1.3 Competition between EF and OFF Interactions; 2.1.4 Edge-Edge (EE) Interactions; 2.2 Three-Dimensional Aromatic Structures; 2.2.1 Aryl . . . Aryl Embrace Interactions; 2.2.2 Design of Heteroaromatic Inclusion Hosts; 2.3 Endo, Endo-Facial Dimers; 2.3.1 The Basic P4AE Interaction Motif; 2.3.2 Discrete Endo,Endo-Facial Dimers; 2.3.3 Aggregated Endo,Endo-Facial Dimers; 2.4 Multiply Halogenated Heteroaromatic Molecules; 2.4.1 The p-Halogen Dimer (PHD) Interaction 2.4.2 The PHD Unit in Staircase Inclusion Structures 2.4.3 The PHD Unit in Layer Structures; 2.4.4 Switch from Endo,Endo-Facial Dimer to PHD Unit; 2.5 Expansion of the Endo,Endo-Facial Dimer; 2.5.1 Penannular Guest Enclosure; 2.5.2 Types of Molecular Pens; 2.6 (EF)₆ Brick-Like Building Blocks; 2.6.1 Phenylated Heteroaromatic Molecules; 2.6.2 Packing of the Bricks; 2.6.3 Different Inclusion Families and Their Convergence; 2.7 Other Novel Multiple Edge-Face Assemblies; 2.7.1 The (EF)₂ Handclasp Interaction; 2.7.2 Formation of Hexameric Inclusion Capsules 2.7.3 Formation of Hexameric Hydrate Clusters 2.8 Other Types of Aryl-Aryl Contacts; 2.8.1 Different OFF Packing Geometries; 2.8.2 Exo, Endo-Facial OFF Interactions; 2.8.3 Exo,Exo-Facial OFF Interactions; 2.8.4 Swivel Interactions; 2.9 Conclusions; Acknowledgments; References; 3 CH-p and p-p Interactions as Contributors to the Guest Binding in Reversible Inclusion and Encapsulation Complexes; 3.1 Introduction; 3.1.1 Theoretical Considerations of Aromatic-Aromatic (p-p) Interactions and CH-p Interactions 3.2 Probing Aromatic-Aromatic (p-p) Interactions and CH-p Interactions with Solid-State Structures of Reversible Inclusion and Encapsulation Complexes

Sommario/riassunto

Crystal engineers aim to control the way molecules aggregate in the crystalline phase and are therefore concerned with crystal structure prediction, polymorphism, and discovering the relative importance of different types of intermolecular forces and their influence on molecular structure. In order to design crystal structures, knowledge of the types, strengths, and nature of possible intermolecular interactions is essential. Non-covalent interactions involving p-systems is a theme that is under extensive investigation as these interactions can be inductors for the assembly of a vast array of
