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| Nota di contenuto | Contents; 1 Introduction and historical background; 1.1 Introduction; 1.2 Definitions; 1.2.1 Polymorphism; 1.2.2 Pseudopolymorphism, solvates, and hydrates; 1.2.3 Conventions for naming polymorphs; 1.3 Is this material polymorphic?; 1.3.1 Occurrence of polymorphism; 1.3.2 Literature sources of polymorphic compounds; 1.3.3 Polymorphic compounds in the Cambridge Structural Database; 1.3.4 Powder Diffraction File; 1.3.5 Patent literature; 1.3.6 Polymorphism of elements and inorganic compounds; 1.3.7 Polymorphism in macromolecular crystals; 1.4 Historical perspective 1.5 Commercial/industrial importance of polymorphism-some additional comments 2 Fundamentals; 2.1 Introduction; 2.2 Thermodynamics of polymorphic molecular crystals; 2.2.1 The Phase Rule; 2.2.2 Thermodynamic relations in polymorphs; 2.2.3 Energy vs temperature diagrams-the Gibbs free energy; 2.2.4 Enantiotropism and monotropism; 2.2.5 Phase diagrams in terms of pressure and temperature; 2.2.6 Heat-of-transition rule; 2.2.7 Heat-of-fusion rule; |

2.2.8 Entropy-of-fusion rule; 2.2.9 Heat-capacity rule; 2.2.10 Density rule; 2.2.11 Infrared rule
2.3 Kinetic factors determining the formation of polymorphic modifications
2.4 Structural fundamentals; 2.4.1 Form vs habit; 2.4.2 Structural characterization and comparison of polymorphic systems; 2.4.3 Presentation of polymorphic structures for comparison; 3 Controlling the polymorphic form obtained; 3.1 General considerations; 3.2 Aggregation and nucleation; 3.3 Thermodynamic vs kinetic crystallization conditions; 3.4 Monotropism, enantiotropism, and crystallization strategy; 3.5 Concomitant polymorphs; 3.5.1 Crystallization methods and conditions
3.5.2 Examples of different classes of compounds
3.5.3 The structural approach; 3.6 Disappearing polymorphs; 3.7 Control of polymorphic crystallization by design; 4 Analytical techniques for studying and characterizing polymorphs; 4.1 Introduction; 4.2 Optical/hot stage microscopy; 4.3 Thermal methods; 4.4 X-ray crystallography; 4.5 Infrared spectroscopy; 4.6 Raman spectroscopy; 4.7 Solid state nuclear magnetic resonance (SSNMR) spectroscopy; 4.8 Scanning electron microscopy; 4.9 Atomic force microscopy (AFM) and scanning tunnelling microscopy (STM); 4.10 Density measurements
4.11 New technologies and 'hyphenated techniques'
4.12 Are two samples polymorphs of the same compound?; 4.13 Concluding remarks; 5 Conformational polymorphism: intra- and intermolecular energetics; 5.1 Introduction; 5.2 Molecular shape and energetics; 5.3 Intermolecular interactions and energetics; 5.4 The search for examples of conformational polymorphism; 5.5 Presenting and comparing conformational polymorphs; 5.6 Some examples of conformational polymorphism; 5.7 What are conformational polymorphs good for?; 5.8 Computational studies of the energetics of polymorphic systems
5.9 Some exemplary studies of conformational polymorphism

Sommario/riassunto

This book deals with polymorphism - the existence of different solid structures of the same chemical entity (for example graphite and diamond, both composed of carbon) which provide ideal systems for investigating the relationship between the structure and properties of a wide variety of materials. - ;Polymorphism - the multiplicity of structures or forms - is a term that is used in many disciplines. In chemistry it refers to the existence of more than one crystal structure for a particular chemical substance. The properties of a substance are determined by its composition and by its structure
