Pharmaceutical Salts And Co Crystals Rsc Drug Discovery

This one-stop reference systematically covers key aspects in early drug development that are directly relevant to the discovery phase and are required for first-in-human studies. Its broad scope brings together critical knowledge from many disciplines, ranging from process technology to pharmacology to intellectual property issues. After introducing the overall early development workflow, the critical steps of early drug development are described in a sequential and enabling order: the availability of the drug substance and that of the drug product, the prediction of pharmacokinetics and -dynamics, as well as that of drug safety. The final section focuses on intellectual property aspects during early clinical development. The emphasis throughout is on recent case studies to exemplify salient points, resulting in an abundance of practice-oriented information that is usually not available from other sources. Aimed at medicinal chemists in industry as well as academia, this invaluable reference enables readers to understand and navigate the challenges in developing clinical candidate molecules that can be successfully used in phase one clinical trials.

This comprehensive up-to-date guide and information source is an instructive companion for all scientists involved in research and development of drugs and, in particular, of pharmaceutical dosage forms. The editors have taken care to address every conceivable aspect of the preparation of pharmaceutical salts and present the necessary theoretical foundations as well as a wealth of detailed practical experience in the choice of pharmaceutically active salts. Altogether, the contributions reflect the multidisciplinary nature of the science involved in selection of suitable salt forms for new drug products.

This book is important because it is the first textbook in an area that has become very popular in recent times. There are around 250 research groups in crystal engineering worldwide today. The subject has been researched for around 40 years but there is still no textbook at the level of senior undergraduates and beginning PhD students. This book is expected to fill this gap. The writing style is simple, with an adequate number of exercises and problems, and the diagrams are easy to understand. This book consists major areas of the subject, including organic crystals and co-ordination polymers, and can easily form the basis of a 30 to 40 lecture course for senior undergraduates.

This unique book focuses on the currently 'hot topic' of Pharmaceutical Salts and Co-crystals. Combining both reports of the latest academic research and comprehensive overviews of basic principles, with more applied contributions from selected experts in industry.

In the last three decades, revolutionary achievements have taken place in nutraceutical and functional food research including the introduction of a number of cutting-edge dietary supplements supported by human clinical trials and strong patents. Novel manufacturing technologies including unique extraction processes, bioavailability improvements, etc.

For the last decade, the topics of organic crystal chemistry have become diversified, and each topic has been substantially advanced in concert with the rapid development of various analytical and measurement techniques for solid-state organic materials. The aim of this book is to systematically summarize and record the recent notable advances in various topics of organic crystal chemistry involving liquid crystals and organic—inorganic hybrid materials that have been achieved mainly in the last 5 years or so. The authors are invited members of the Division of Organic Crystals, The Chemical Society of Japan (CSJ), and prominent invited experts from abroad. This edited volume is planned to be published periodically, at least every 5 years, with contributions by prominent authors in Japan and from abroad.

Focusing on developments from the past 10-15 years, this volume presents an objective overview of the research in charge density analysis. The most promising methodologies are included, in addition to powerful interpretative tools and a survey of important areas of research.

This volume provides readers with the basic principles and fundamentals of extrusion technology and a detailed description of the practical applications of a variety of extrusion processes, including various pharma grade extruders. In addition, the downstream production of films, pellets and tablets, for example, for oral and other delivery routes, are presented and discussed utilizing melt extrusion. This book is the first of its kind that discusses extensively the well-developed science of extrusion technology as applied to pharmaceutical drug product development and manufacturing. By covering a wide range of relevant topics, the text brings together all technical information necessary to develop and market pharmaceutical dosage forms that meet current quality and regulatory requirements. As extrusion technology continues to be refined further, usage of extruder systems and the array of applications will continue to expand, but the core technologies will remain the same.

In this volume, contributions covering the theoretical and practical aspects of multicomponent crystals provide a timely and contemporary overview of the state-of-the-art of this vital aspect of crystal engineering/materials science. With a solid foundation in fundamentals, multi-component crystals can be formed, for example, to enhance pharmaceutical properties of drugs, for the specific control of optical responses to external stimuli and to assemble molecules to allow chemical reactions that are generally intractable following conventional methods. ContentsPharmaceutical co-crystals: crystal engineering and applicationsPharmaceutical multi-component crystals: improving the efficacy of anti-tuberculous agentsQualitative and quantitative crystal engineering of multi-functional co-crystals Control of photochromism in N-salicylideneaniline by crystal engineeringQuinoline derivatives for multi-component crystals: principles and applicationsN-oxides in multi-component crystals and in bottom-up synthesis and applicationsMulti-component crystals and non-ambient conditions Co-crystals for solid-state reactivity and thermal expansionSolution co-crystallisation and its applicationsThe salt-co-crystal continuum in halogen-bonded systemsLarge horizontal displacements of benzene-benzene stacking interactions in co-crystalsSimultaneous halogen and hydrogen bonding to carbonyl and thiacarbonylfuctionality Crystal chemistry of the isomeric N,N’-bis(pyridin-n-ylmethyl)-ethanediimides, n = 2, 3 or 4Solute:solvent interactions mediated by main group element (lone-pair)??????(aryl) interactions

Crystallization is an important purification process used in a broad range of industries, including pharmaceuticals, foods, and bulk chemicals. In recent years, molecular modeling has emerged as a useful tool in the analysis and solution of problems associated with crystallization. Modeling allows more focused experimentation based on structural and energetic calculations instead of intuition and trial and error. This book offers a general introduction to molecular modeling techniques and their application in crystallization. After explaining the basic concepts of molecular modeling...
and crystallization, the book discusses how modeling techniques are used to solve a variety of practical problems related to crystal size, shape, internal structure, and properties. With chapters written by leading experts and an emphasis on problem solving, this book will appeal to scientists, engineers, and graduate students involved in research and the production of crystalline materials.

This book summarizes and records the recent notable advances in diverse topics in organic crystal chemistry, which has made substantial progress along with the rapid development of a variety of analysis and measurement techniques for solid organic materials. This review book is one of the volumes that are published periodically on this theme. The previous volume, published in 2015, systematically summarized the remarkable progress in assorted topics of organic crystal chemistry using organic solids and organic–inorganic hybrid materials during the previous 5 years, and it has been widely read. The present volume also shows the progress of organic solid chemistry in the last 5 years, with contributions mainly by invited members of the Division of Organic Crystal Chemistry of the Chemical Society of Japan (CSJ), together with prominent invited authors from countries other than Japan.

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.

The book Recrystallization in Materials Processing shows selected results obtained during the last few years by researchers worked on recrystallization-related issues. These researchers offer their knowledge from a range of scientific disciplines, such as materials science, metallurgy and pharmacology. The authors emphasize that the progress in this particular field of scientific research is possible today due to coordinated efforts of many research groups that work in materials science, chemistry, physics, pharmacology, and other sciences. Thus, it is possible to perform a detailed analysis of the scientific problem. The analysis starts from the selection of appropriate techniques and methods of characterization. It is then combined with the development of new tools in diagnostics, and it finished with physical modeling of phenomena.

Hardbound. A substantial amount of recent research has revealed that an understanding of weak intermolecular interactions is a most important priority in the chemical sciences today. One of the many advantages to ensue from such an understanding is that improved methods for the prediction and design of organic crystal structures have become possible. Concurrently, strategies for crystal engineering have advanced to such an extent to warrant the publication of this book in which the author reviews and evaluates past developments, and comments on future possibilities. The book is intended for three distinct groups of scientists: organic chemists and materials scientists who are now coordinating their efforts in designing molecular crystals for a variety of physical and chemical applications; physical and theoretical chemists who are concerned with intermolecular interactions in organic solids; crystallographers who attempt to search for patterns in crys

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Each chapter has three types of learning aids for students: open-ended questions, multiple-choice questions, and quantitative problems. There is an average of about 50 per chapter. There are also a number of worked examples in the chapters, averaging over 5 per chapter, and almost 600 photos and line drawings.

From crystal structure prediction to totally empirical screening, the quest for new crystal forms has become one of the most challenging issues in the solid state science and particularly in the pharmaceutical world. In this context, multi-component crystalline materials like co-crystals have received renewed interest as they offer the prospect of optimized physical properties. As illustrated in this first book, entirely dedicated to this emerging class of pharmaceutical compounds, the outcome of such endeavours into crystal engineering have demonstrated clear impacts on production, marketing and intellectual property protection of active pharmaceutical ingredients (APIs). Indeed, co-crystallization influences relevant physico-chemical parameters (such as solubility, dissolution rate, chemical stability, melting point, hygroscopicity, a) and often offers solids with properties superior to those of the free drug. Combining both reports of the latest research and comprehensive overviews of basic principles, with contributions from selected experts in both academia and industry, this unique book is an essential reference, ideal for pharmaceutical development scientists and graduate students in pharmaceutical science.

Oral lipid-based formulations are attracting considerable attention due to their capacity to facilitate gastrointestinal absorption and reduce or eliminate the effect of food on the absorption of poorly water-soluble, lipophilic drugs. Despite the obvious and demonstrated utility of these formulations for addressing a persistent and growing problem

The two-word title of this book can only give an indication about its content and approach to the subject it deals with. In the course of time, the term has gradually become somewhat blurred. The reason is easy to see: similar problems are now more and more frequently studied by different branches of natural science. The term "mixed crystals" has acquired specific connotations in physics, chemistry, biology, and geology. One and the same term can now serve as a name for things which are either not quite the same or sometimes quite different. And this is precisely what happened to the two words in the title of the book. One of them, the term "crystal", for which crystallography had an unambiguous definition, is now employed by biologists to describe the structure of cell membranes and by chemists who use it to denote degrees of polymer crystallinity. "Crystal" has thus become a broad term that can help describe any solid, or just a condensed state of a substance, if the solid has a sufficient degree of order in the arrangement of its components. But the book is called "Mixed Crystals". The other word in its title, the adjective "mixed", has also developed several meanings. It is now thought up to be both homogeneous and heterogeneous systems, that is, to crystals composed of different molecules and also to solids that are a mixture of crys that exist in different structures.

Sterile Drug Products: Formulation, Packaging, Manufacturing, and Quality teaches the basic principles of the development and manufacture of high quality sterile dosage forms. The author has 38 years of experience in the development and manufacture of sterile dosage forms, including solutions, suspensions, ophthalmics and freeze dried products. This book is based on the courses he has delivered for over three decades, to over 3000 participants, and is intended to remain relevant for the indefinite future even as new technologies and new applications of old technologies become common. This is an ideal reference book for those working directly and indirectly with sterile dosage forms, be it product development (formulation, package, process, analytical), manufacturing, quality control, quality assurance, regulatory, purchasing, or
project management. This book is also intended as an educational resource for the pharmaceutical and biopharmaceutical industry and pharmacy schools, providing basic knowledge and principles in four main areas of parenteral science and technology: Product development, including formulation, packaging, and process development. Manufacturing, including basic teaching on all the primary unit operations involved in preparation of sterile products and the underlying importance of contamination control. Quality and regulatory, including the application of good manufacturing practice regulations, aseptic processing guidelines, and unique quality control testing methods for the sterile dosage form Clinical aspects, including administration, potential hazards, and biopharmaceutics of sterile products in a clinical setting. Multi-component crystalline systems or co-crystals have received tremendous attention from academia and industry alike in the past decade. Applications of co-crystals are varied and are likely to positively impact a wide range of industries dealing with molecular solids. Co-crystallization has been used to improve the properties and performance of materials from pharmaceuticals to energetic materials, as well as for separation of compounds. This book combines co-crystal applications of commercial and practical interest from diverse fields to in a single volume. It also examines effective structural design of co-crystals, and provides insights into practical synthesis and characterization techniques. Providing a useful resource for postgraduate students new to applied co-crystal research and crystal engineering, it will also be of interest to established researchers in academia or industry. This book aims to provide the reader with a working knowledge of the various means of controlling the solubility or dissolution rate of a drug or other solute in an aqueous medium. The book begins with the factors which govern solubility in general and then looks at aqueous solubility in particular, including the properties of liquid mixtures and the thermodynamics of solutions formed from mixing two components. The bulk of the book is then devoted to techniques for altering solubility and dissolution rate of organic compounds in aqueous media. It discusses in detail the most commonly used solubility enhancers: buffers, cosolvents, surfactants, and complexants. Each chapter is self-contained and emphasizes the details for applying the techniques. Edited by one of the leading experts in the field, this handbook emphasizes why solid-state issues are important, which approaches should be taken to avoid problems and exploit the opportunities offered by solid state properties in the pharmaceutical and agricultural industries. With its practical approach, this is at once a guideline for development chemists just entering the field as well as a high-quality source of reference material for specialists in the pharmaceutical and chemical industry, structural chemists, physicochemists, crystallographers, inorganic chemists, and patent departments. This volume is intended to provide the reader with a breadth of understanding regarding the many challenges faced with the formulation of poorly water-soluble drugs as well as in-depth knowledge in the critical areas of development with these compounds. Further, this book is designed to provide practical guidance for overcoming formulation challenges toward the end goal of improving drug therapies with poorly water-soluble drugs. Enhancing solubility via formulation intervention is a unique opportunity in which formulation scientists can enable drug therapies by creating viable medicines from seemingly undeletable molecules. With the ever increasing number of poorly water-soluble compounds entering development, the role of the formulation scientist is growing in importance. Also, knowledge of the advanced analytical, formulation, and process development technologies as well as specific regulatory considerations related to the formulation of these compounds is increasing in value. Ideally, this book will serve as a useful tool in the education of current and future generations of scientists, and in this context contribute toward providing patients with new and better medicines. Atomically precise metal nanocluster research has emerged as a new frontier. This book serves as an introduction to metal nanoclusters protected by ligands. The authors have summarized the synthesis principles and methods, the characterization methods and new physicochemical properties, and some potential applications. By pursuing atomic precision, such nanocluster materials provide unprecedented opportunities for establishing precise relationships between the atomic-level structures and the properties. The book should be accessible to senior undergraduate and graduate students, researchers in various fields (e.g., chemistry, physics, materials, biomedicine, and engineering), R&D scientists, and science policy makers. This volume focuses on how to increase the efficiency of drug discovery and development. It is written by experienced discovery scientists from diverse disciplines, including chemistry, drug metabolism, and development sciences. The volume details in silico, in vitro, and in vivo tools for prediction, measurement, and application of compound properties to select and improve potential drug candidates. Our understanding of the properties of materials, from drugs and proteins to catalysts and ceramics, is almost always based on structural information. This book describes the new developments in the realm of powder diffraction which make it possible for scientists to obtain such information even from polycrystalline materials. Written and edited by experts active in the field, and covering both the fundamental and applied aspects of structure solution from powder diffraction data, this book guides both novices and experienced practitioners alike through the maze of possibilities. The crystalline state is the most commonly used essential solid active pharmaceutical ingredient (API). The characterization of pharmaceutical crystals encompasses many scientific disciplines, but the core is crystal structure analysis which reveals the molecular structure of essential pharmaceutical compounds. Crystal structure analysis provides important structural information related to the API's wide range of physicochemical properties, such as solubility, stability, tablet performance, color, and hygroscopicity. This book entitled "Pharmaceutical Crystals" focuses on the relationship between crystal structure and physicochemical properties. In particular, the new crystal structure of pharmaceutical compounds involving multi-component crystals, such as co-crystals, salts, and hydrates, and polymorph crystals are reported. Such crystal structures were investigated in the latest studies that combined morphology, spectroscopic, theoretical calculation, and thermal analysis with crystallographic study. This book highlights the importance of crystal structure information in many areas of pharmaceutical science and presents current trends in the structure–property study of pharmaceutical crystals. The Guest Editors of this book hope the readers enjoy a wide variety of recent studies on Pharmaceutical Crystals. 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. In the last two decades, there has been a sharp rise in the interest in polymorphic systems, as an intrinsically interesting phenomenon and as an increasingly important component in the development and marketing of a variety of materials based on organic molecules (e.g. pharmaceuticals, dyes and pigments, explosives, etc.). This book summarizes and brings up to date the current knowledge and understanding of polymorphism of molecular crystals, and concentrates it in one comprehensive source. The book will be an invaluable reference for students, researchers, and professionals in the field. "Polymorphism in the Pharmaceutical Industry - Solid Form and Drug Development" highlights the relevance of polymorphism in modern pharmaceutical chemistry, with a focus on quality by design (QbD) concepts. It covers all important issues by way of case studies, ranging from properties and crystallization, via thermodynamics, analytics and theoretical modelling right up to patent issues. As such, the book underscores the importance of solid-state chemistry within chemical and pharmaceutical development. It
emphasizes why solid-state issues are important, the approaches needed to avoid problems and the opportunities offered by solid-
state properties. The authors include true polymorphs as well as solvates and hydrates, while providing information on
physicochemical properties, crystallization thermodynamics, quantum-mechanical modelling, and up-scaling. Important analytical
tools to characterize solid-state forms and to quantify mixtures are summarized, and case studies on solid-state development
processes in industry are also provided. Written by acknowledged experts in the field, this is a high-quality reference for
researchers, project managers and quality assurance managers in pharmaceutical, agrochemical and fine chemical companies as
well as for academics and newcomers to organic solid-state chemistry.

A guide to the latest industry principles for optimizing the production of solid state active pharmaceutical ingredients Solid State
Development and Processing of Pharmaceutical Molecules is an authoritative guide that covers the entire pharmaceutical value
chain. The authors—noted experts on the topic—examine the importance of the solid state form of chemical and biological drugs and review the development, production, quality control, formulation, and stability of medicines. The book explores the most recent
trends in the digitization and automation of the pharmaceutical production processes that reflect the need for consistent high
quality. It also includes information on relevant regulatory and intellectual property considerations. This resource is aimed at professionals in the pharmaceutical industry and offers an in-depth examination of the commercially relevant issues facing developers, producers and distributors of drug substances. This important book: Provides a guide for the effective development of solid drug forms Compares different characterization methods for solid state APIs Offers a resource for understanding efficient production methods for solid state forms of chemical and biological drugs Includes information on automation, process control, and machine learning as an integral part of the development and production workflows Covers in detail the regulatory and quality control aspects of drug development Written for medicinal chemists, pharmaceutical industry professionals, pharma engineers, solid state chemists, chemical engineers, Solid State Development and Processing of Pharmaceutical Molecules reviews information on the solid state of active pharmaceutical ingredients for their efficient development and production. An important resource that puts the focus on understanding and handling of organic crystals in drug development Since a majority of pharmaceutical solid-state materials are organic crystals, their handling and processing are critical aspects of drug development. Pharmaceutical Crystals: Science and Engineering offers an introduction to and thorough coverage of organic crystals, and explores the essential role they play in drug development and manufacturing. Written contributions from leading researchers and practitioners in the field, this vital resource provides the fundamental knowledge and explains the connection between pharmaceutically relevant properties and the structure of a crystal. Comprehensive in scope, the text covers a range of topics including: crystallization, molecular interactions, polymorphism, analytical methods, processing, and chemical stability. The authors clearly show how to find solutions for pharmaceutical form selection and crystallization processes. Designed to be an accessible guide, this book represents a valuable resource for improving the drug development process of small drug molecules. This important text: Includes the most important aspects of solid-state organic chemistry and its role in drug development Offers solutions for pharmaceutical form selection and crystallization processes Contains a balance between the scientific fundamental and pharmaceutical applications Presents coverage of crystallography, molecular interactions, polymorphism, analytical methods, processing, and chemical stability Written for both practicing pharmaceutical scientists, engineers, and senior undergraduate and graduate students studying pharmaceutical solid-state materials, Pharmaceutical Crystals: Science and Engineering is a reference and textbook for understanding, producing, analyzing, and designing organic crystals which is an imperative skill to master for anyone working in the field. Presents a detailed discussion of important solid-state properties, methods, and applications of solid-state analysis Illustrates the various phases or forms that solids can assume and discussessvarious issues related to the relative stability of solid forms and tendencies to undergo transformation Covers key methods of solid state analysis including X-ray powder diffraction, thermal analysis, microscopy, spectroscopy, and solid state NMR Reviews critical physical attributes of pharmaceutical materials, mainly related to drug substances, including particle size/surface area, hygroscopicity, mechanical properties, solubility, and physical and chemical stability Showcases the application of solid state material science in rational selection of drug solid forms, analysis of various solid forms within drug substance and the drug product, and pharmaceutical product development Introduces appropriate manufacturing and control procedures using Quality by Design, and other strategies that lead to safe and effective products with a minimum of resources and time The COSMO-RS technique is a novel method for predicting the thermodynamic properties of pure and mixed fluids which are important in many areas, ranging from chemical engineering to drug design. COSMO-RS, From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design is about this novel technology, which has recently proven to be the most reliable and efficient tool for the prediction of vapour-liquid equilibria. In contrast to group contribution methods, which depend on an extremely large number of experimental data, COSMO-RS calculates the thermodynamic data from molecular surface polarity distributions, resulting from quantum chemical calculations of the individual compounds in the mixture. In this book, the author cleverly combines a vivid overview of the partly demanding theoretical steps with a deeper analysis of their scientific background and justification. Aimed at theoretical chemists, computational chemists, physical chemists, chemical engineers, thermodynamicists as well as students, academic and industrial experts, COSMO-
RS, From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design provides a novel viewpoint to anyone looking to gain more insight into the theory and potential of the unique method, COSMO-RS. The only book currently available on COSMO-RS technique Provides a novel viewpoint for the scientific understanding and for the practical quantitative treatment of fluid phase thermodynamics Includes illustrative examples of the COSMOTHERM program Crystal engineering - where the myriad of intermolecular forces operating in the solid-state are employed to design new nano- and functional materials - is a key new technology with implications for catalysis, pharmaceuticals, synthesis and materials science. Frontiers in Crystal Engineering gathers personal perspectives, from international specialists working in molecular aspects of crystal engineering, on the practical and theoretical challenges of the discipline, and future prospects. These demonstrate the approaches that are being used to tackle the problems associated with the complexity, design and functionality of crystalline molecular solids. Topics include * how intermolecular forces direct and sustain
crystal structures * functional engineering and design elements * coordination polymers and network structures * applications in green and pharmaceutical chemistry Frontiers in Crystal Engineering is a useful guide to this exciting new discipline for both entrants to the field as well as established practitioners, and for those working in crystallography, medicinal and pharmaceutical sciences, solid-state chemistry, and materials and nanotechnology.

"Presents a comprehensive examination of polymorphic behavior in pharmaceutical development-demonstrating with clear, practical examples how to navigate complicated crystal structures. Edited by the recipient of the American Association of Pharmaceutical Scientists’ 1998 Research Achievement Award in Analysis and Pharmaceutical Quality."

In nearly all process industries, crystallization is used at some stage as a method of production, purification or recovery of solid materials. In recent years, a number of new applications have also come to rely on crystallization processes such as the crystallization of nano and amorphous materials. The articles in this book have been contributed by some of the most respected researchers in this area and cover the frontier areas of research and developments in crystallization processes. Divided into three sections, this book provides the latest research developments in many aspects of crystallization including the crystallization of biological macromolecules and pharmaceutical compounds, the crystallization of nanomaterials and the crystallization of amorphous and glassy materials. This book is of interest to both fundamental research and practicing scientists and will prove invaluable to all chemical engineers and industrial chemists in process industries, as well as crystallization workers and students in industry and academia.

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