Determination Of Solubility Parameters And Thermodynamic

Macromolecular Solutions: Solvent-Property Relationships in Polymers is a collection of papers presented at a symposium on Macromolecular Solutions, held New York City on August 23-28, 1981, sponsored by the American Chemical Society at its 182nd national meeting. This book is composed of 19 chapters and begins with discussions on the concept, application, and analysis of solubility parameters of polymers. The succeeding chapters deal with the role of solubility parameters in polymer coating design and stress cracking of nylon. Considerable chapters are devoted to the preparation, properties, reactions, and analysis of various polymers and copolymers. These topics are followed by surveys of the polymer-surfactant interaction effect on polymer solution properties and the effects of methanol-gasoline mixtures on elastomers. The final chapters describe the residual solvent content effect on dissolution kinetics of polymers; the application of excimer fluorescence to measure polymer-solvent interactions; and a general procedure for the calculation of thermodynamic properties of polymer solutions. This book will be of great value to polymer chemists, manufacturers, and researchers.

During recent years the number of poorly soluble drug candidate has risen sharply and the formulation of poorly soluble compounds for oral delivery now presents one of the most frequent and greatest challenges to formulation scientist in pharmaceutical industry. One of the most attractive options for increasing the release rate is improvement of the solubility and dissolution rate utilizing amorphous forms of the drug and solid dispersion system. In this project GSK-X (BSC II) was employed as a drug model for the formulation of solid dispersion. The aim of this study was to determine the miscibility of drug model GSK-X (BSCII) and excipients to predict if glass solutions are likely to form when drug and polymer are formulated in a solid dispersion system. -- Estimation of drug/excipient miscibility was performed using Hansen solubility parameters (HSPs) which were determined experimentally by IGC and computationally using the HSPiP software. Due to poor agreement between the two sets of data, the solid dispersion-forming excipients were chosen on matching the HSPs determined experimentally by IGC. -- Solid state and physical chemical characterization of formulations prepared with 'good' polymers identified as poly(ethylene oxide) and poly(vinyl acetate) and 'bad' polymers such as poly(vinyl pyrrolidone) and Eudragit E 100 obtained by XRPD, MDSC and dissolution showed that experimental results were not in agreement with solubility parameter predictions. It was observed that the manufacturing process and the drug and polymer properties may limit the development of a successful formulation.

Organic solvents represent a class of compounds whose utility is central to industrial and academic chemistry. The impact of solvents in everyday products such as paints, surface coatings, adhesives, pharmaceuticals and cleaning products is enormous, and there is therefore much interest in their use.

This volume is divided into two parts. Part 1 provides and authoritative review of the science and technology of solvents and related issues. The topics covered are solvency and its measurement, flammability, health and toxicology, environmental issues, legislative information, transport, storage, recovery and disposal, and a review of solvent applications. Part 2 provides reliable, up- to-date data, based on information provided by manufacturers and suppliers and is presented as a database of over 350 solvent products, subdivided by solvent group. The data are also presented in key parameter tables, covering boiling points, melting points, evaporation information, vapor pressure, flash points, solubility parameters, auto ignition temperatures, and names and addresses of manufacturers, with trade names. In recent years there has been increased interest in health and safety, environmental issues and aspects of the legislative control of chemicals, including solvents, and the choice of a given solvent has therefore become more complex. The Directory of Solvents aims to provide in one place a broad spread of physico-chemical data, together with transport, safety, environmental and classification information provided by major European and U.S. suppliers and manufacturers of industrial organic solvents.

Directory of Solvents

Determination of the Solubility Parameters for Non-polar Amorphous and Crystalline Polymers by an Equilibrium Swelling Method

Gas-Adsorption Chromatography

Solubility and Solvents for Conservation Problems

Solubility Parameters and Gas Chromatography

The U.S. Coast Guard set out to determine three-dimensional solubility parameters for several new materials. The final approach employed three measures of responses to exposure of material to each of 56 solvents of diverse solubility parameters. The intent was to identify the best measure for this purpose in terms of ease of conducting the test and its statistical reliability. The responses measured were: visual observation of changes, volume increase, and weight gain. Weight gain proved to be the best measure of the three, providing the greatest amount of information with the least experimental error. Tests were conducted on: butyl rubber, chlorobutyl rubber, "three-ply" chlorinated polyethylene, Viton A (copolymer), Viton B (terpolymer), and Teflon. Tests conducted for 24 h gave essentially the same results as those conducted for one week. No three-dimensional solubility parameter could be obtained for Teflon, because of its minimal interaction throughout the solubility parameter space. Aqueous solubility is one of the major challenges in the early stages of drug discovery. One of the most common and effective methods for enhancing solubility is the addition of an organic solvent to the aqueous solution. Along with an introduction to cosolvency models, the Handbook of Solubility Data for Pharmaceuticals provides an extensive database of solubility for pharmaceuticals in mono solvents and binary solvents. Aqueous solubility data can be found in the Handbook of Aqueous Solubility Data by

Samuel Yalkowsky and Yan He. Visit www.crcpress.com for more information. In addition to the experimental efforts to measure the solubility of drugs in mono and mixed solvents, this book discusses the advantages and limitations of a number of mathematical models used to predict the solubility in mono or mixed solvent systems. It covers the pharmaceutical cosolvents and other organic solvents that are used in syntheses, separations, and other pharmaceutical processes. The solutes featured include the available data for official drugs, drug candidates, precursors of drugs, metabolites, and degradation products of pharmaceuticals. The author also presents the solubilities of amino acids since they play an important role in peptide drug properties. Collecting drug solubilities in various cosolvents, this time-saving handbook includes the mixtures and model constants needed to predict undetermined solubilities. It describes mathematical models that enable data to be derived and provides estimates on how drugs are likely to behave in a given cosolvent. A software program and associated user manual are available on the author's website.

"Molecular Gels: Materials with Self-Assembled Fibrillar Networks" is a comprehensive treatise on gelators, especially low molecular-mass gelators and the properties of their gels. The structures and modes of formation of the self-assembled fibrillar networks (SAFINs) that immobilize the liquid components of the gels are discussed experimentally and theoretically. The spectroscopic, rheological, and structural features of the different classes of low molecular-mass gelators are also presented. Many examples of the application of the principal analytical techniques for investigation of molecular gels (including SANS, SAXS, WAXS, UV-vis absorption, fluorescence and CD spectroscopies, scanning electron, transmission electron and optical microscopies, and molecular modeling) are presented didactically and in-depth, as are several of the theories of the stages of aggregation of individual low molecular-mass gelator molecules leading to SAFINs. Several actual and potential applications of molecular gels in disparate fields (from silicate replication of nanostructures to art conservation) are described. Special emphasis is placed on perspectives for future developments. This book is an invaluable resource for researchers and practitioners either already researching self-assembly and soft matter or new to the area. Those who will find the book useful include chemists, engineers, spectroscopists, physicists, biologists, theoreticians, and materials scientists.

Theory and Practice

Interdisciplinary Approach to Liquid Lubricant Technology

COSMO-RS

Materials with Self-Assembled Fibrillar Networks

from ADME to Toxicity Optimization

parameter estimates based on the two simplifying assumptions differed by no more than 0.2 hildebrands, an

increment equal to the presumed inherent error of estimation. These data, then, indicate that solubility parameters and, thus, cohesive energies of crystalline organic solids can be determined from their solubilities in London solvents.

This is the first book to present a topical overview of the research and development of microbial polyesters. Comprehensive and amply illustrated, it covers the * biosynthesis * structure * properties * applications of these biodegradable and biocompatible thermoplastics. The book provides the reader with the necessary background to understand the nature and mechanism of biological polymerization. It unites aspects from both the biological and polymer sciences and is a typical modern example of the analysis of biological macromolecules.

Carbon in Earth's fluid envelopes - the atmosphere, biosphere, and hydrosphere, plays a fundamental role in our planet's climate system and a central role in biology, the environment, and the economy of earth system. The source and original quantity of carbon in our planet is uncertain, as are the identities and relative importance of early chemical processes associated with planetary differentiation. Numerous lines of evidence point to the early and continuing exchange of substantial carbon between Earth's surface and its interior, including diamonds, carbon-rich mantle-derived magmas, carbonate rocks in subduction zones and springs carrying deeply sourced carbon-bearing gases. Thus, there is little doubt that a substantial amount of carbon resides in our planet's interior. Yet, while we know it must be present, carbon's forms, transformations and movements at conditions relevant to the interiors of Earth and other planets remain uncertain and untapped. Volume highlights include: - Reviews key, general topics, such as carbonate minerals, the deep carbon cycle, and carbon in magmas or fluids - Describes new results at the frontiers of the field with presenting results on carbon in minerals, melts, and fluids at extreme conditions of planetary interiors - Brings together emerging insights into carbon's forms, transformations and movements through study of the dynamics, structure, stability and reactivity of carbon-based natural materials - Reviews emerging new insights into the properties of allied substances that carry carbon, into the rates of chemical and physical transformations, and into the complex interactions between moving fluids, magmas, and rocks to the interiors of Earth and other planets - Spans the various chemical redox states of carbon, from reduced hydrocarbons to zero-valent diamond and graphite to oxidized CO2 and carbonates - Captures and synthesizes the exciting results of recent, focused efforts in an emerging scientific discipline - Reports advances over the last decade that have led to a major leap forward in our understanding of carbon science - Compiles the range of methods that can be tapped tap from the deep carbon community, which includes experimentalists, first principles theorists, thermodynamic modelers and geodynamicists - Represents a reference point for future deep carbon science research Carbon in Planetary Interiors will be a valuable resource for researchers and students who study the Earth's interior. The topics of this volume are interdisciplinary, and

therefore will be useful to professionals from a wide variety of fields in the Earth Sciences, such as mineral physics, petrology, geochemistry, experimentalists, first principles theorists, thermodynamics, material science, chemistry, geophysics and geodynamics.

Solvent-Property Relationships in Polymers

Proceedings of the Ninth International Symposium on Cyclodextrins

Solubility of Polysaccharides

Hdbk OF SOLUBILITY PARAMETERS OTHER COHESION PARAMETERS

Determination of the Relationship Between Permeation Rates and Solubility Parameter Differences for Selected Protective Glove/solvent and Boot/solvent Combinations

Now available for the first time, this valuable reference presents polymer solubility parameters and various polymer-liquid interaction parameters in an easy-to-use form. It critically evaluates and comprehensively compiles data from original sources. It presents these quantities polymer-by-polymer, alphabetically by polymer common chemical name, fully cross-referenced by systematic chemical names, alternative names and trade names. This one-of-a-kind handbook summarizes the relationship between the various quantities and their methods of determination. This resource is an absolute must for all who are interested in the chemical industry, specifically polymer chemistry, chemical engineering, applied chemistry, and physical chemistry.

The 3rd edition of this important dictionary offers more than 12,000 entries with expanded encyclopaedic-style definitions making this major reference work invaluable to practitioners, researchers and students working in the area of polymer science and technology. This new edition now includes entries on computer simulation and modeling, surface and interfacial properties and their characterization, functional and smart polymers. New and controlled architectures of polymers, especially dendrimers and controlled radical polymerization are also covered.

The continued search for rapid, efficient and cost-effective means of analytical measurement has introduced supercritical fluids into the field of analytical chemistry. Two areas are common: supercritical fluid chroma tography and supercritical fluid extraction. Both seek to exploit the unique properties of a gas at temperatures and pressures above the critical point. The most common supercritical fluid is carbon dioxide, employed because of its low critical temperature (31 °C), inertness, purity, non-toxicity and cheapness. Alternative supercritical fluids are also used and often in conjunction with modifiers. The combined gas-like mass transfer and liquid-like solvating characteristics have been used for improved chroma tographic separation and faster sample preparation. Supercritical fluid chromatography (SFC) is complementary to gas chro matography (GC) and high performance liquid chromatography (HPLC), providing higher efficiency than HPLC, together with the ability to analyse thermally labile and high molecular weight analytes. Both packed and open tubular columns can be employed, providing the capability to analyse a wide range of sample types. In addition, flame ionization detection can be used, thus providing 'universal' detection.

Macromolecular Solutions

Applications of Supercritical Fluids in Industrial Analysis

Handbook of Solubility Data for Pharmaceuticals

ON THE APPLICATION OF REGULAR SOLUTION THEORY TO THE ESTIMATION OF SOLUBILITY PARAMETERS OF CRYSTALLINE ORGANIC COMPOUNDS FROM SOLUBILITY DATA.

A User's Handbook, Second Edition

* Guidelines are provided on the reliability of various methods, as well as information for selecting the appropriate technique. * Unique coverage of the whole range of solubility measurements. * Very useful for investigators interested in embarking upon solubility measurements.

The CRC Handbook of Solubility Parameters and Other Cohesion Parameters, Second Edition, which includes 17 new sections and 40 new data tables, incorporates information from a vast amount of material published over the last ten years. The volume is based on a bibliography of 2,900 reports, including 1,200 new citations. The detailed, careful construction of the handbook develops the concept of solubility parameters from empirical, thermodynamic, and molecular points of view and demonstrates their application to liquid, gas, solid, and polymer systems.

High-precision cleaning is required across a wide range of sectors, including aerospace, defense, medical device manufacturing, pharmaceutical processing, semiconductor/electronics, etc. Cleaning parts and surfaces with solvents is simple, effective and low-cost. Although health and safety and environmental concerns come into play with the use of solvents, this book explores how safe and compliant solvent-based cleaning techniques can be implemented. A key to this is the selection of the right solvent. The author also examines a range of newer "green" solvent cleaning options. This book supplies scientific fundamentals and practical guidance supported by real-world examples. Durkee explains the three principal methods of solvent selection: matching of solubility parameters, reduction of potential for smog formation, and matching of physical properties. He also provides guidance on the safe use of aerosols, wipe-cleaning techniques, solvent stabilization, economics, and many other topics. A compendium of blend rules is included, covering the physical, chemical, and environmental properties of solvents. Three methods explained in detail for substitution of suitable solvents for those unsuitable for any reason: toxic solvents don't have to be tolerated; this volume explains how to do better Enables users to make informed judgments about their selection of cleaning solvents for specific applications, including solvent replacement decisions Explains how to plan and implement solvent cleaning systems that are effective, economical and compliant with regulations

Handbook of Poylmer-Liquid Interaction Parameters and Solubility Parameters

Molecular Gels

Experimental Determination of Solubility Parameter Values for the Acetone-dichloromethane Binary System

Determination of Solubility Parameter of Polymer by Microwave Absorption in Waveguide

Determination of Solubility Parameters of New Suit Materials

Sugars, with a scientific term as saccharides, are involved in various aspects in the lives of human beings, including the sense of taste, energy for daily life, etc. Recent development in polysaccharides, as well as the background knowledge in this field, further deepens insight into their roles as healthy supplements. In this book, the principles on polysaccharides' solubility and structure, methodologies and application of polysaccharides have been reviewed. The chapters in this book include the relationship between structure and solubility of polysaccharide, the experimental and computational researches on polysaccharide solubility and the common polysaccharide, which may further aid scholars and researchers in regard to solubility of polysaccharides, methodologies and modification.

This volume contains the proceedings of the Ninth International Symposium on Cyclodextrins, held in Santiago de Compostela, Spain, May 31 - June 3, 1998. The papers collected represent a summary of the last two years' achievements

in the application of cyclodextrins in such diverse fields as pharmaceuticals, biotechnology, textiles, chromatography and environmental sciences. Highlights: Chiral selection of chemicals, nuclear waste management, cyclodextrins in nasal drug delivery, cyclodextrins in pulmonary drug delivery, cyclodextrins as pharmaceutical excipients, pharmacokinetics, stabilization of drugs by cyclodextrins, structural characterization of cyclodextrin complexes by nuclear magnetic resonance and molecular modeling, artificial receptors, large cyclodextrins, cyclodextrins as enzyme models, new cyclodextrin derivatives and potentials. Audience: This book will be of interest to researchers whose work involves biotechnology, pharmaceuticals, food and chemicals and chromatographic methods, as well as fundamental cyclodextrin research.
Properties of Polymers: Their Correlation with Chemical Structure; Their Numerical Estimation and Prediction from Additive Group Contributions summarizes the latest developments regarding polymers, their properties in relation to chemical structure, and methods for estimating and predicting numerical properties from chemical structure. In particular, it examines polymer electrical properties, magnetic properties, and mechanical properties, as well as their crystallization and environmental behavior and failure. The rheological properties of polymer melts and polymer solutions are also considered. Organized into seven parts encompassing 27 chapters, this book begins with an overview of polymer science and engineering, including the typology of polymers and their properties. It then turns to a discussion of thermophysical properties, from transition temperatures to volumetric and calorimetric properties, along with the cohesive aspects and conformation statistics. It also introduces the reader to the behavior of polymers in electromagnetic and mechanical fields of force. The book covers the quantities that influence the transport of heat, momentum, and matter, particularly heat conductivity, viscosity, and diffusivity; properties that control the chemical stability and breakdown of polymers; and polymer properties as an integral concept, with emphasis on processing and product properties. Readers will find tables that give valuable (numerical) data on polymers and include a survey of the group contributions (increments) of almost every additive function considered. This book is a valuable resource for anyone working on practical problems in the field of polymers, including organic chemists, chemical engineers, polymer processers, polymer technologists, and both graduate and PhD students.

Regular and Related Solutions

Santiago de Compostela, Spain, May 31–June 3, 1998

Theoretical and Experimental Determination of the Hansen Solubility Parameters as Miscibility Predictors for the Formulation of Solid Dispersions

Regulation of Tissue Oxygenation, Second Edition

Hansen Solubility Parameters in Practice

This volume offers a comprehensive guide on the theory and practice of amorphous solid dispersions (ASD) for handling challenges associated with poorly soluble drugs. In twenty-three inclusive chapters, the book examines thermodynamics and kinetics of the amorphous state and amorphous solid dispersions, ASD technologies, excipients for stabilizing amorphous solid dispersions such as polymers, and ASD manufacturing technologies, including spray drying, hot melt extrusion, fluid bed layering and solvent-controlled micro-precipitation technology (MBP). Each technology is illustrated

by specific case studies. In addition, dedicated sections cover analytical tools and technologies for characterization of amorphous solid dispersions, the prediction of long-term stability, and the development of suitable dissolution methods and regulatory aspects. The book also highlights future technologies on the horizon, such as supercritical fluid processing, mesoporous silica, KinetiSol®, and the use of non-salt-forming organic acids and amino acids for the stabilization of amorphous systems. Amorphous Solid Dispersions: Theory and Practice is a valuable reference to pharmaceutical scientists interested in developing bioavailable and therapeutically effective formulations of poorly soluble molecules in order to advance these technologies and develop better medicines for the future.

This presentation describes various aspects of the regulation of tissue oxygenation, including the roles of the circulatory system, respiratory system, and blood, the carrier of oxygen within these components of the cardiorespiratory system. The respiratory system takes oxygen from the atmosphere and transports it by diffusion from the air in the alveoli to the blood flowing through the pulmonary capillaries. The cardiovascular system then moves the oxygenated blood from the heart to the microcirculation of the various organs by convection, where oxygen is released from hemoglobin in the red blood cells and moves to the parenchymal cells of each tissue by diffusion. Oxygen that has diffused into cells is then utilized in the mitochondria to produce adenosine triphosphate (ATP), the energy currency of all cells. The mitochondria are able to produce ATP until the oxygen tension or PO2 on the cell surface falls to a critical level of about 4–5 mm Hg. Thus, in order to meet the energetic needs of cells, it is important to maintain a continuous supply of oxygen to the mitochondria at or above the critical PO2 . In order to accomplish this desired outcome, the cardiorespiratory system, including the blood, must be capable of regulation to ensure survival of all tissues under a wide range of circumstances. The purpose of this presentation is to provide basic information about the operation and regulation of the cardiovascular and respiratory systems, as well as the properties of the blood and parenchymal cells, so that a fundamental understanding of the regulation of tissue oxygenation is achieved.

Hansen solubility parameters (HSPs) are used to predict molecular affinities, solubility, and solubility-related phenomena. Revised and updated throughout, Hansen Solubility Parameters: A User's Handbook, Second Edition features the three Hansen solubility parameters for over 1200 chemicals and correlations for over 400 materials including polymers, inorganic salts, and biological materials. To update his groundbreaking handbook with the latest advances and perspectives, Charles M. Hansen has invited five renowned experts to share their work, theories, and practical applications involving HSPs. New discussions include a new statistical thermodynamics approach for confirming existing HSPs and how they fit into other thermodynamic theories for polymer solutions. Entirely new chapters examine the prediction of environmental stress cracking as well as absorption and diffusion in polymers. Highlighting recent findings on interactions with DNA, the treatment of biological materials also includes skin tissue, proteins, natural fibers, and cholesterol. The book also covers the latest applications of HSPs, such as ozone-safe “designer” solvents, protective clothing, drug delivery systems, and petroleum applications. Presenting a comprehensive survey of the theoretical and practical aspects of HSPs, Hansen Solubility Parameters, Second Edition concludes with a detailed discussion on the necessary research, future directions, and potential applications for which HSPs can provide a useful means of prediction

in areas such as biological materials, controlled release applications, nanotechnology, and self-assembly.
Determination of Miscibility of Pvc/polymer Blends by Three-dimensional Solubility Parameters
Hansen Solubility Parameters
The Solubility of Gases, Liquids, and Solids
From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design
An Experimental Determination of the Ability of Nonpolar and Polar Solubility Parameters to Locate and Distinguish Optimum Aprotic Extraction Solvents

Hansen Solubility ParametersA User's Handbook, Second EditionCRC Press

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

Of the thousands of novel compounds that a drug discovery project team invents and that bind to the therapeutic target, typically only a fraction of these have sufficient ADME/Tox properties to become a drug product. Understanding ADME/Tox is critical for all drug researchers, owing to its increasing importance in advancing high quality candidates to clinical studies and the processes of drug discovery. If the properties are weak, the candidate will have a high risk of failure or be less desirable as a drug product. This book is a tool and resource for scientists engaged in, or preparing for, the selection and optimization process. The authors describe how properties affect in vivo pharmacological activity and impact in vitro assays. Individual drug-like properties are discussed from a practical point of view, such as solubility, permeability and metabolic stability, with regard to fundamental understanding, applications of property data in drug discovery and examples of structural

*modifications that have achieved improved property performance. The authors also review various methods for the screening (high throughput), diagnosis (medium throughput) and in-depth (low throughput) analysis of drug properties. * Serves as an essential working handbook aimed at scientists and students in medicinal chemistry * Provides practical, step-by-step guidance on property fundamentals, effects, structure-property relationships, and structure modification strategies * Discusses improvements in pharmacokinetics from a practical chemist's standpoint*

Drug-like Properties: Concepts, Structure Design and Methods

Solubility Parameters and Evaporation Rate Analysis in Organic Residue Characterization

The Solubility of Nonelectrolytes

Polymer Science Dictionary

Carbon in Earth's Interior

The proceedings of a conference of liquid lubricant technology are presented. The subjects discussed are: (1) requirements and functions of liquid lubricants, (2) mineral oils, (3) greases, (4) theory of rheology, (5) mechanics and thermodynamics in lubrication, (6) environmental capability of liquid lubricants, and (7) wear corrosion and erosion.

CRC Handbook of Solubility Parameters and Other Cohesion Parameters

Cleaning with Solvents: Science and Technology

Supplement to Determination of Liquid-mixture Solubility Parameters and Interaction Energy Densities

The Experimental Determination of Solubilities

Determination and Prediction of Asphaltene Instability at Reservoir Conditions Using Solubility Parameter Technique