Determination Of Surface Pka Values Of Surface Confined

The importance of solid base catalysts has come to be recognized for their environmentally benign qualities, and much significant progress has been made over the past two decades in catalytic materials and solid base-catalyzed reactions. The book is focused on the solid base. Because of the advantages over liquid bases, the use of solid base catalysts in organic synthesis is expanding. Solid bases are easier to dispose than liquid bases, separation and recovery of products, catalysts and solvents are less difficult, and they are non-corrosive. Furthermore, base-catalyzed reactions can be performed without using solvents and even in the gas phase, opening up more possibilities for discovering novel reaction systems. Using numerous examples, the present volume describes the remarkable role solid base catalysis can play, given the ever increasing worldwide importance of "green" chemistry. The reader will obtain an overall view of solid base catalysis and gain insight into the versatility of the reactions to which solid base catalysts can be utilized. The concept and significance of solid base catalysis are discussed, followed by descriptions of various methods for the characterization of solid bases, including

spectroscopic methods and test reactions. The preparation and properties of base materials are presented in detail, with the two final chapters devoted to surveying the variety of reactions catalyzed by solid bases.

First published in 1996, liposomes have become an important model in fundamental biomembrane research, including biophysical, biochemical, and cell biological studies of membranes and cell function. They are thoroughly studied in several applications, such as drug delivery systems in medical applications and as controlled release systems, microencapsulating media, signal carriers, support matrices, and solubilizers in other applications. While medical applications have been extensively reviewed in recent literature, there is a need for easily accessible information on applications for liposomes beyond pharmacology and medicine. The Handbook of Nonmedical Applications of Liposomes fills this void.This unique new handbook series presents recent developments in the use of liposomes in many scientific disciplines, from studies on the origin of life, protein function, and vesicle shapes, to applications in cosmetics, diagnostics, ecology, bioreclamation, and the food industry. In these volumes many of the top experts contribute extensive reviews of their work.

This is the first volume on adsorption using green adsorbents and is written by international

contributors who are the leading experts in the adsorption field. The first volume provides an overview of fundamentals and design of adsorption processes. For people who are new to the field, the book starts by two overview chapters presenting the principles and properties of wastewater treatment and adsorption processes. The book also provides a comprehensive source of knowledge on acid-base properties of biosorbents. It discusses fractal-like kinetic models for fluid-solid adsorption, reports on the chemical characterization of oxidized activated carbons for metal removal, and the use of magnetic biosorbents in water treatment. Furthermore, the thermodynamic properties of metals adsorption by green adsorbents, and biosorption of polycyclic aromatic hydrocarbons and organic pollutants are reviewed, and finally the recent trends and impact of nanomaterials as green adsorbent and potential catalysts for environmental applications are summarized. The audience for this book includes students, environmentalists, engineers, water scientists, civil and industrial personnel who wish to specialize in adsorption technology. Academically, this book will be of use to students in chemical and environmental engineering who wish to learn about adsorption and its fundamentals. It has also been compiled for practicing engineers who wish to know about recent developments on adsorbent materials in order to promote further research toward

improving and developing newer adsorbents and processes for the efficient removal of pollutants from industrial effluents. It is hoped that the book will serve as a readable and useful presentation not only for undergraduate and postgraduate students but also for the water scientists and engineers and as a convenient reference handbook in the form of numerous recent examples and appended information.

Nanomaterials - substances smaller than 100 nanometers in size - have been added in recent years to an increasing numbers of consumer products used in day-to-day life; in food packaging, medical devices, pharmaceuticals, cosmetics, odor-resistant textiles and household appliances. The extensive application of nanomaterials in a wide range of products for human use poses a potential for toxicity risk to human health and the environment. Such adverse effects of nanomaterials on human health have triggered the development of a new scientific discipline known as “nanotoxicity” – the study of the toxicity of nanomaterials. Nanotoxicity: From in vivo and in vitro Models to Health Risks provides up-to-date state-of-the-art information presented by recognized experts in this emerging new field in toxicology. It discusses the safety evaluation of nanomaterials in foods, drugs, medical devices, cosmetics and other regulated products and its use in risk analysis for potential regulatory use.

Topics covered include: biomarkers for nanotoxicity assessment nanotoxicity assessment by gene expression analysis in vivo and in vitro models for nanotoxicity testing mechanisms of nanotoxicity pharmakokinetics of nanomaterials nanotoxicity of foods including food processing, food packaging and food safety nanotoxicity of drugs including drug development and drug delivery nanotoxicity of cosmetics and consumer products health and environmental impact of nanotoxicity safety evaluation of nanomaterials regulatory impact of nanomaterials Nanotoxicity: From in vivo and in vitro Models to Health Risks is a valuable authoritative source of information for readers from a wide range of disciplines such as toxicology, pharmacology, drug toxicity and food and environmental sciences. The book will be useful to the research community in academia, industry, hospitals and government, as well as to government regulators and risk assessors of foods, drugs and environmental and agricultural products.

This text focuses on the physics of fluid transport in micro- and nanofabricated liquid-phase systems, with consideration of gas bubbles, solid particles, and macromolecules. This text was designed with the goal of bringing together several areas that are often taught separately - namely, fluid mechanics, electrodynamics, and interfacial chemistry and electrochemistry - with a focused goal of preparing

the modern microfluidics researcher to analyse and model continuum fluid mechanical systems encountered when working with micro- and nanofabricated devices. This text serves as a useful reference for practising researchers but is designed primarily for classroom instruction. Worked sample problems are included throughout to assist the student, and exercises at the end of each chapter help facilitate class learning.

Determination of Organic Structures by Physical Methods, Volume 1 focuses on the processes, methodologies, principles, and approaches involved in the determination of organic structures by physical methods, including infrared light absorption, thermodynamic properties, Raman spectra, and kinetics. The selection first elaborates on the phase properties of small molecules, equilibrium and dynamic properties of large molecules, and optical rotation. Discussions focus on simple acyclic compounds, carbohydrates, steroids, diffusion, viscosity, osmotic pressure, sedimentation velocity, melting and boiling points, and molar volume. The book then examines ultraviolet and visible light absorption, infrared light absorption, Raman spectra, and the theory of magnetic susceptibility. Concerns cover applications to the study of organic compounds, applications to the determination of structure, determination of thermodynamic properties, and experimental methods and

evaluation of data. The text ponders on wave-mechanical theory, reaction kinetics, and dissociation constants, including dissociation of molecular addition compounds, principles of reaction kinetics, and valence-bond treatment of aromatic systems. The selection is a valuable source of data for researchers interested in the determination of organic structures by physical methods.

This 24th volume continues in the tradition of its predecessors, presenting authoritative, interdisciplinary coverage of contemporary topics in the field of carbon chemistry and physics. With contributions by leading international experts, this volume: describes pitch polymerization kinetics during mesophase formation and the constitution of coexisting phases in mesophase pitch during heat treatment; elucidates the mechanism of mesophase formation and pitch polymerization kinetics after mesophase formation; examines the importance of physical, solid-state, electro- and analytical chemistry in the study of carbon surfaces; discusses the theoretical background for the thermal conductivity of diamonds, single crystal diamonds and chemically-vapour-deposited diamond films; and explains the chemistry involved in the commercial fabrication and use of needle coke.

A comprehensive overview of current empirical valence bond (EVB) theory and applications, one of the most powerful tools for studying chemical

processes in the condensed phase and in enzymes. Discusses the application of EVB models to a broad range of molecular systems of chemical and biological interest, including reaction dynamics, design of artificial catalysts, and the study of complex biological problems Edited by a rising star in the field of computational enzymology Foreword by Nobel laureate Arieh Warshel, who first developed the EVB approach

This book presents chemical analyses of the most pressing waste, pollution, and resource problems for the undergraduate or graduate student. Its distinctive holistic approach provides a solid introduction to theory as well as a practical laboratory manual detailing beginning and advanced experimental applications. It presents laboratory procedures at microscale conditions, for minimum waste and maximum economy.

This book provides a description of the generalized two layer surface complexation model, data treatment procedures, and thermodynamic constants for sorption of metal cations and anions on gibbsite, the most common form of aluminum oxide found in nature and one of the most abundant minerals in soils, sediments, and natural waters. The book provides a synopsis of aluminum oxide forms and a clearly defined nomenclature. Compilations of available data for sorption of metal cations and anions on gibbsite are presented, and the results of

surface complexation model fitting of these data are given. The consistency of the thermodynamic surface complexation constants extracted from the data is examined through development of linear free energy relationships which are also used to predict thermodynamic constants for ions for which insufficient data are available to extract constants. The book concludes with a comparison of constants extracted from data for sorption on gibbsite with those determined previously for hydrous ferric oxide (HFO), hydrous manganese oxide (HMO), and goethite. The overall objective of this book is the development and presentation of an internally consistent thermodynamic database for sorption of inorganic cations and anions on gibbsite, an abundant and reactive mineral in soils, sediments, and aquatic systems. Its surface has a high affinity for sorption of metal cations and anions, including radionuclides. The gibbsite database will enable simulation and prediction of the influence of sorption on the fate of these chemical species in natural systems and treatment processes in which aluminum oxides are abundant. It thus will help to advance the practical application of surface complexation modeling.

In the first volume of this series, the structures of protein molecules were described, together with computational methods linking sequence data to folded structure and function. The determination of

protein structure by nuclear magnetic resonance spectroscopy was also presented. Volume 2 begins by continuing the theme of protein structure with an outline of methods of crystallographic structure determination. Subsequent chapters describe various strucure-related properties of proteins. This book provides a valuable contribution to those new to the field of protein science as well as to those already expert in the field.

The bestselling reference on environmental microbiology—now in a new edition This is the long-awaited and much-anticipated revision of the bestselling text and reference. Based on the latest information and investigative techniques from molecular biology and genetics, this Second Edition offers an in-depth examination of the role of microbiological processes related to environmental deterioration with an emphasis on the detection and control of environmental contaminants. Its goal is to further our understanding of the complex microbial processes underlying environmental degradation, its detection and control, and ultimately, its prevention. Features new to this edition include: A completely new organization with topics such as pathogens in developing countries, effects of genetically modified crops on microbial communities, and transformations of toxic metals Comprehensive coverage of key topics such as bacteria in the greenhouse and low-energy waste treatment New coverage relating core

book content to local, regional, and global environmental problems Environmental Microbiology, Second Edition is essential reading for environmental microbiologists and engineers, general environmental scientists, chemists, and chemical engineers who are interested in key current subjects in environmental microbiology. It is also appropriate as a textbook for courses in environmental science, chemistry, engineering, and microbial ecology at the advanced undergraduate and graduate levels.

European Cooperation in Science and Technology (COST) supports the collaboration of nationally-funded science and technology research through the creation of networks. COST is the longest-running European framework enhancing cooperation among researchers, engineers and scholars across Europe. The COST Action CM1103 “Structure-based drug design for diagnosis and treatment of neurological diseases: dissecting and modulating complex function in the monoaminergic systems of the brain” is a good example of the advances possible through interdisciplinary collaboration on difficult problems. COST Action CM1103 brought together 28 research groups from 18 countries to collaborate for four years on multi-target drug design for complex neuropathologies. The interdisciplinary expertise of the members is spans the range from computational enzymology to human studies, providing outstanding

opportunities for the interdisciplinary development of trainees, and is reflected in the articles in this e-book. This Research Topic covers progress in multi-target drug design for the complex neuropathologies of the monoamine system that are apparent, for example, in Alzheimer's disease. After a mini-review to introduce the topic of multi-target drug design, the other articles review the Research topic from their own perspective, two from computational approaches, three from medicinal chemistry, two from molecular pharmacology, and two from studies in whole brain. This multi-faceted approach describes new compounds, new methodology, and advances in the basic science of understanding the brain. This Ebook is based upon work from COST Action (CM1103 "Structure-based drug design for diagnosis and treatment of neurological diseases: dissecting and modulating complex function in the monoaminergic systems of the brain"), supported by COST (European Cooperation in Science and Technology). COST (European Cooperation in Science and Technology) is a pan-European intergovernmental framework. Its mission is to enable break-through scientific and technological developments leading to new concepts and products and thereby contribute to strengthening Europe's research and innovation capacities. It allows researchers, engineers and scholars to jointly develop their own ideas and take new initiatives

across all fields of science and technology, while promoting multi- and interdisciplinary approaches. COST aims at fostering a better integration of less research intensive countries to the knowledge hubs of the European Research Area. The COST Association, an International not-for-profit Association under Belgian Law, integrates all management, governing and administrative functions necessary for the operation of the framework. The COST Association has currently 36 Member Countries. www.cost.eu

This text offers an overview of the recent theoretical and practical results achieved in gas-solid, liquid-solid and gas-liquid adsorption research.

This edited book, is a collection of 20 articles describing the recent advancements in the application of microbial technology for sustainable development of agriculture and environment. This book covers many aspects like agricultural nanotechnology, promising applications of biofuels production by algae, advancements and application of microbial keratinase, biocontrol agents, plant growth promoting rhizobacteria, bacterial siderophore, use of microbes in detoxifying organophosphate pesticides, bio-surfactants, biofilms, bioremediation degradation of phenol and phenolic compounds and bioprospecting of endophytes. This book intends to bring the latest research advancements and technologies in the

area of microbial technology in one platform, providing the readers an up-to-date view on the area. This book would serve as an excellent reference book for researchers and students in the agricultural, environmental and microbiology fields. Colloid and interface science dealt with nanoscale objects for nearly a century before the term nanotechnology was coined. An interdisciplinary field, it bridges the macroscopic world and the small world of atoms and molecules. Colloid and Interface Chemistry for Nanotechnology is a collection of manuscripts reflecting the activities of research teams that have been involved in the networking project Colloid and Interface Chemistry for Nanotechnology (2006–2011), Action D43, the European Science Foundation. The project was a part of the intergovernmental framework for Cooperation in Science and Technology (COST), allowing the coordination of nationally funded research across Europe. With contributions by leading experts, this book covers a wide range of topics. Chapters are grouped into three sections: "Nanoparticle Synthesis and Characterization," "New Experimental Tools and Interpretation," and "Nanocolloidal Dispersions and Interfaces." The topics covered belong to six basic research areas: (1) The synthesis of nanostructured materials of well-defined size and function; (2) Analytical methods and tools for control and characterization of synthesized

nanomaterials; (3) Self-assembly of nanomaterials, such as microemulsions and micelles, and their applications; (4) Bioinspired nanostructured materials—structure, properties, and applications; (5) Design of active, soft functional interfaces with unique properties for sensors, catalysts, and biomedical assays; and (6) Nanoscale elements in soft nanoscale devices for applications in analytical and biomedical sciences. This book describes highlights in nanotechnology based on state-of-the-art principles in colloid and interface science, demonstrating how great progress in the various branches of nanotechnology can be achieved. The application of these principles allows for the development of new experimental and theoretical tools.

Molecular processes in nature affect human health, the availability of resources and the Earth's climate. Molecular modelling is a powerful and versatile toolbox that complements experimental data and provides insights where direct observation is not currently possible. Molecular Modeling of Geochemical Reactions: An Introduction applies computational chemistry to geochemical problems. Chapters focus on geochemical applications in aqueous, petroleum, organic, environmental, bio- and isotope geochemistry, covering the fundamental theory, practical guidance on applying techniques, and extensive literature reviews in numerous

geochemical sub-disciplines. Topics covered include: • Theory and Methods of Computational Chemistry • Force Field Application and Development • Computational Spectroscopy • Thermodynamics • Structure Determination • Geochemical Kinetics This book will be of interest to graduate students and researchers looking to understand geochemical processes on a molecular level. Novice practitioners of molecular modelling, experienced computational chemists, and experimentalists seeking to understand this field will all find information and knowledge of use in their research.

To provide an interdisciplinary readership with the necessary toolkit to work with micro- and nanofluidics, this book provides basic theory, fundamentals of microfabrication, advanced fabrication methods, device characterization methods and detailed examples of applications of nanofluidics devices and systems. Case studies describing fabrication of complex micro- and nanoscale systems help the reader gain a practical understanding of developing and fabricating such systems. The resulting work covers the fundamentals, processes and applied challenges of functional engineered nanofluidic systems for a variety of different applications, including discussions of lab-on-chip, bio-related applications and emerging technologies for energy and environmental

engineering. The fundamentals of micro- and nanofluidic systems and micro- and nanofabrication techniques provide readers from a variety of academic backgrounds with the understanding required to develop new systems and applications. Case studies introduce and illustrate state-of-the-art applications across areas, including lab-on-chip, energy and bio-based applications. Prakash and Yeom provide readers with an essential toolkit to take micro- and nanofluidic applications out of the research lab and into commercial and laboratory applications.

Chemistry of Powder Production focuses on the solid-state chemistry of powder materials and relates this to the structure, properties and preparation, and characterization techniques for these important industrial products. Additionally, the properties of the particles are discussed in relation to their surface structure and characteristics. This book describes the fundamentals of statistical methods for measuring the characteristics of particles. New advanced materials being developed in powder technology manufacturing techniques are also emphasised, including powdered materials for advanced ceramics as well as magnetic and pigment materials.

The characterization of materials and phenomena has historically been the principal limitation to the development in each area of science. Once what we

are observing is well defined, a theoretical analysis rapidly follows. Modern theories of chemical bonding did not evolve until the methods of analytical chemistry had progressed to a point where the bulk stoichiometry of chemical compounds was firmly established. The great progress made during this century in understanding chemistry has followed directly from the development of an analytical chemistry based on the Dalton assumption of multiple proportions. It has only become apparent in recent years that the extension of our understanding of materials hinges on their non-stoichiometric nature. The world of non-Daltonian chemistry is very poorly understood at present because of our lack of ability to precisely characterize it. The emergence of materials science has only just occurred with our recognition of effects, which have been thought previously to be minor variations from ideality, as the principal phenomena controlling properties. The next step in the historical evolution of materials science must be the development of tools to characterize the often subtle phenomena which determine properties of materials. The various discussions of instrumental techniques presented in this book are excellent summaries for the state-of-the-art of materials characterization at this rather critical stage of materials science. The application of the tools described here, and those yet to be developed, holds the key to the development of this infant into a

mature science.

"Kinetics and Dynamics" on molecular modeling of dynamic processes opens with an introductory overview before discussing approaches to reactivity of small systems in the gas phase. Then it examines studies of systems of increasing complexity up to the dynamics of DNA. This title has interdisciplinary character presenting wherever possible an interplay between the theory and the experiment. It provides basic information as well as the details of theory and examples of its application to experimentalists and theoreticians interested in modeling of dynamic processes in chemical and biochemical systems. All contributing authors are renowned experts in their fields and topics covered in this volume represent the forefront of today's science.

Describes the supramolecular properties of molecular assemblies that contain a solid phase, offering an integrated approach to measurement and addressibility. * Offers an integrated approach to measurement and addressibility. * Features case studies describing the major devices developed using this technology. * The prospects for the future of interfacial supramolecular assemblies are considered.

A handbook on syntheses and properties, production processes, and applications of maleic anhydride and maleic anhydride derived products – all in one text. This handbook provides a comprehensive overview

of maleic anhydride chemistry and applications from the professional perspective. With chapters written by leading R&D scientists from the chemical industry, and edited by the Vice President and ASI Technology Chief at Ashland Specialty Ingredients (ASI), Dr. Osama M. Musa, readers will find a unique perspective and summary of the latest advancements in the field of maleic anhydride science. Maleic anhydride is produced industrially on large scale (10E3 kt/annum). Its rich chemistry makes it an important raw material for numerous products and processes (e.g. for applications in polymers and coatings), many of which are covered in this handbook for the first time in a comprehensive manner. The broad scope spans topics ranging from production techniques (including topics such as processes, catalysis, trouble-shooting), synthesis and properties of small and polymeric maleic anhydride based compounds (focusing on industrially relevant compounds as well as emerging areas of importance) and in-depth and broad discussions of commercial maleic anhydride based applications.

The International Scientific Conference “FarEastCon” took place on October 1-4, 2019 in Vladivostok, Russian Federation. This collection presents papers reflecting recent advances in the field of materials engineering and technologies for production and processing in the different areas of

modern manufacturing.

Organized nanoassemblies of inorganic nanoparticles and organic molecules are building blocks of nanodevices, whether they are designed to perform molecular level computing, sense the environment or improve the catalytic properties of a material. The key to creation of these hybrid nanostructures lies in understanding the chemistry at a fundamental level. This book serves as a reference book for researchers by providing fundamental understanding of many nanoscopic materials.

This book describes the role modern pharmaceutical analysis plays in the development of new drugs. Detailed information is provided as to how the quality of drug products is assured from the point of discovery until the patient uses the drug. Coverage includes state-of-the-art topics such as analytics for combinatorial chemistry and high-throughput screening, formulation development, stability studies, international regulatory aspects and documentation, and future technologies that are likely to impact the field. Emphasis is placed on current, easy-to-follow methods that readers can apply in their laboratories. No book has effectively replaced the very popular text, Pharmaceutical Analysis, that was edited in the 1960s by Tak Higuchi. This book will fill that gap with an up-to-date treatment that is both handy and authoritative.

Separation Methods in Drug Synthesis and

Purification, Second Edition, Volume Eight, provides an updated on the analytical techniques used in drug synthesis and purification. Unlike other books on either separation science or drug synthesis, this volume combines the two to explain the basic principles and comparisons of each separation technique. New sections to this volume include enantiomer separation using capillary electrophoresis (CE) and capillary electro-chromatography, the computer simulation of chromatographic separation for accelerating method development, the application of chromatography and capillary electrophoresis used as surrogates for biological processes, and new developments in the established techniques of chromatography and preparative methods. Features descriptions and applications of all separation methods used in the pharmaceutical industry Written by the leading scientists in their respective fields, providing solutions for a wide range of industrial separation problems encountered within the pharmaceutical industry Thoroughly updated with brand new separation science techniques and the latest developments in the established techniques of chromatography

Determination of Surface PKa Values of Surface-confined Molecules Derivatized with PH-sensitive Pendant GroupsDetermination of Surface PKa Values of Surface-Confined Molecules Derivitized

with PH-Sensitive Pendant Groups

Agricultural and food industry waste materials have been an important feedstock for activated carbon production for many years. In the development of cleaner energy production and utilization processes, new advanced carbon materials with enhanced properties have been studied. Techniques to tailor pore structure and surface chemistry can produce better carbon materials for energy storage, electrode materials, and selective adsorption of pollutants. This book surveys available waste materials and processes for carbon production and then reviews the recent developments in the use of carbon materials for energy storage, as catalyst supports, and for environmental applications.

This book is a printed edition of the Special Issue "Immobilized Biocatalysts" that was published in Catalysts

This first book to focus on the use of SPMs to actively manipulate molecules and nanostructures on surfaces goes way beyond conventional treatments of scanning microscopy merely for imaging purposes. It reviews recent progress in the use of SPMs on such soft materials as polymers, with a particular emphasis on chemical discrimination, mechanical properties, tip-induced reactions and manipulations, as well as their nanoscale electrical properties. Detailing the practical application potential of this hot topic, this

book is of great interest to specialists of wide-ranging disciplines, including physicists, chemists, materials scientists, spectroscopy experts, surface scientists, and engineers.

Presented in an easy-to-read form, this book on zeolite catalysis cover all aspects of the subject. It focuses on synthesis, structure, diffusion, deactivation, and industrial applications. This book is an ideal text for courses on catalysis or as a supplementary text for those studying applied or industrial chemistry. It is also a useful resource for anyone who works with zeolites as catalysts in the laboratory, pilot plants, or commercial installations.

Nano/micro-size particles are widely applied in various fields. Among the various particles, silver particles are considered among the most prominent nanomaterials in the biomedical and industrial sectors because of their favorable physical, chemical, and biological characteristics. Thus, numerous studies have been conducted to evaluate their properties and utilize them in various applications, such as diagnostics, anti-bacterial and anti-cancer therapeutics, and optoelectronics. The properties of silver particles are strongly influenced by their size, morphological shape, and surface characteristics, which can be modified by diverse synthetic methods, reducing agents, and stabilizers. This Special Issue provides a range of original contributions detailing the synthesis, modification,

properties, and applications of silver materials. Nine outstanding papers describing examples of the most recent advances in silver nano/microparticles are included. Silver nano/micro-size particles have many potential advantages as next-generation materials in various areas, including nanomedicine. This Special Issue might be helpful to understand the value of silver particles in the biomedical and industrial fields The pKa of a compound describes its acidity or basicity and, therefore, is one of its most important properties. Its value determines what form of the compound—positive ion, negative ion, or neutral species—will be present under different circumstances. This is crucial to the action and detection of the compound as a drug, pollutant, or other active chemical agent. In many cases it is desirable to predict pKa values prior to synthesizing a compound, and enough is now known about the salient features that influence a molecule's acidity to make these predictions. Computational Approaches for the Prediction of pKa Values describes the insights that have been gained on the intrinsic and extrinsic features that influence a molecule's acidity and discusses the computational methods developed to estimate acidity from a compound's molecular structure. The authors examine the strengths and weaknesses of the theoretical techniques and show how they have been used to obtain information about the acidities of different

classes of chemical compounds. The book presents theoretical methods for both general and more specific applications, covering methods for various acids in aqueous solutions—including oxyacids and related compounds, nitrogen acids, inorganic acids, and excited-state acids—as well as acids in nonaqueous solvents. It also considers temperature effects, isotope effects, and other important factors that influence pKa. This book provides a resource for predicting pKa values and understanding the bases for these determinations, which can be helpful in designing better chemicals for future uses.
Provides comprehensive coverage of the chemical interactions among organic and inorganic solids, air, water, microorganisms, and the plant roots in soil
This book focuses on the species and reaction processes of chemicals in soils, with applications to environmental and agricultural issues. Topics range from discussion of fundamental chemical processes to review of properties and reactions of chemicals in the environment. This new edition contains more examples, more illustrations, more details of calculations, and reorganized material within the chapters, including nearly 100 new equations and 51 new figures. Each section also ends with an important concepts overview as well as new questions for readers to answer. Starting with an introduction to the subject, Soil Chemistry, 5th Edition offers in-depth coverage of properties of

elements and molecules; characteristics of chemicals in soils; soil water chemistry; redox reactions in soils; mineralogy and weathering processes in soils; and chemistry of soil clays. The book also provides chapters that examine production and chemistry of soil organic matter; surface properties of soil colloids; adsorption processes in soils; measuring and predicting sorption processes in soils; soil acidity; and salt-affected soils. Provides a basic description of important research and fundamental knowledge in the field of soil chemistry Contains more than 200 references provided in figure and table captions and at the end of the chapters Extensively revised with updated figures and tables Soil Chemistry, 5th Edition is an excellent text for senior-level soil chemistry students.

Whilst following in the footsteps of previous volumes by presenting comprehensive reviews of drug substances and additional materials, this title also heralds a significant expansion of the scope of the series. Traditional contributions will now also be augmented by publication of critical review chapters that summarize information related to the characterization of drug substances and excipients. This change is required to better meet the needs of the pharmaceutical communtiy and to allow the development of a timely vehicle for publishing review materials on this topic. The scope of the Profiles series will encompass review articles and database

compilations that fall within one of the following six broad categories: Physical profiles of drug substances and excipients; Analytical profiles of drug substances and excipients; Drug metabolism and pharmacokinetic profiles of drug substances and excipients; Methodology related to the characterization of drug substances and excipients; Methods of chemical synthesis; and Reviews of the uses and applications for individual drug substances, classes of drug substances, or excipients. * Presents comprehensive reviews covering all aspects of drug development and formulation of drugs * Now encompassing critical review chapters * Meets the information needs of the drug development community

Two methods for in-situ electrochemical measurements of surface pKa values air, reported. The methods are applied to surface-confined monolayers consisting of organomercaptan molecules derivitized with pH-sensitive pendant groups. The first technique relies upon pH-dependent electrostatic binding of redox probe molecules to the charged monolayer surface: the surface concentration of the probe molecules reflects the degree of surface protonation. The second method relates the differential capacitance of the monolayer-modified electrode surface to the surface pKa. The two methods yield essentially identical results and are consistent with a recently developed

theoretical model. The surface pKa values of 4-mercaptopyridine and 4-aminothiophenol are 3. 7 and 5.7, respectively.

During the last two decades, the pharmaceutical industry has been under pressure to reduce development costs and the time needed to bring drugs to market in order to maximize return on investment and bring treatments to patients sooner. To meet these ends, pharmaceutical scientists working in the differing areas of pharmacy, pharmaceutics, and phar