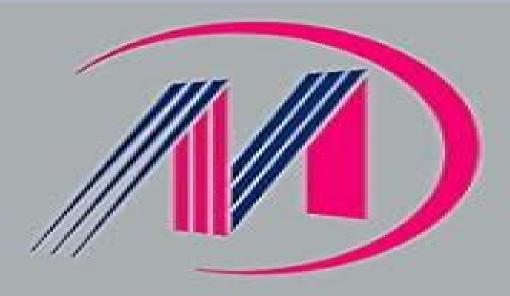


Mass Spectrometry

VOLUME 1

Theory and Ion Chemistry

P. B. ARMENTROUT



EDITORS-IN-CHIEF: Michael L. Gross & Richard M. Caprioli

Encyclopedia Of Mass Spectrometry Theory And Ion Chemistry

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The Encyclopedia of Mass Spectrometry: Theory and ion chemistry Michael L. Gross, R. M. Caprioli, 2003 Encyclopedia of Mass Spectrometry: Theory and ion chemistry, 2003 The Encyclopedia of Mass Spectrometry Michael L. Gross, Wilfried Niessen, R. M. Caprioli, 2006-10-30 Presents information on the biographies of recognized pioneers and innovators in the field of mass spectrometry Highlights over 120 innovators in mass spectrometry including several Nobel Prize winners Discusses instrumentation and their uses also providing interesting information on the careers characters and life stories of the people who did the work Offers unique insight into the careers and personalities of The Encyclopedia of Mass Spectrometry Michael L. Gross, P.B. Armentrout, R. M. luminaries in the field Caprioli, 2003-07-25 This multi volume work provides comprehensive coverage of the full range of topics and techniques in mass spectrometry Techniques methods and applications are described in detail including limitations current problems and areas in which the method does not succeed well The Encyclopedia of Mass Spectrometry Keith A. Nier, Alfred L. Yergey, P. Jane Gale, 2015-07-02 Volume 9 Historical Perspectives Part B Notable People in Mass Spectrometry of The Encyclopedia of Mass Spectrometry briefly reviews the lives and works of many of the major people who carried out this development providing insights into the history of mass spectrometry applications through the personal stories of pioneers and innovators in the field The book presents biographies of notable contributors including Nobel Prize winners J J Thomson Francis W Aston Wolfgang Paul John B Fenn and Koichi Tanaka along with other luminaries in the field including Franz Hillenkamp Catherine Clarke Fenselau Alfred O C Nier and many more discussing not only the instruments and their uses but also providing interesting information on the careers characters and life stories of the people who did the work Highlights over 120 innovators in mass spectrometry including several Nobel Prize winners Discusses instrumentation and their uses also providing interesting information on the careers characters and life stories of the people who did the work Offers unique insight into the careers and personalities of luminaries in the field Coordinates with Volume 9 Historical Perspectives Part A The Development of Mass Spectrometry an overview of mass spectrometry development and progress Ideal reference for those interested in a wide variety of topics including analytical chemistry and chemical analysis amongst The Encyclopedia of Mass Spectrometry, 2015-12-04 Volume 9 Historical Perspectives Part A The Development of others Mass Spectrometry of The Encyclopedia of Mass Spectrometry describes and analyzes the development of many aspects of Mass Spectrometry Beginning with the earliest types of Mass Analyzers Historical Perspectives explores the development of many different forms of analytical processes and methods The work follows various instruments and interfaces to the current state of detectors and computerization It traces the use of Mass Spectrometry across many different disciplines including Organic Chemistry Biochemistry and Proteomics Environmental Mass Spectrometry Forensic Science Imaging Medical Monitoring and Diagnosis Earth and Planetary Sciences and Nuclear Science Finally the book covers the history of

manufacturers and societies as well as the professionals who form the Mass Spectrometry community Also available Volume 9 Historical Perspectives Part B Notable People in Mass Spectrometry briefly reviews the lives and works of many of the major people who carried out this development Preserves the history and development of Mass Spectrometry for use across scientific fields Written and edited by Mass Spectrometry experts Coordinates with Volume 9 Historical Perspectives Part B Notable People in Mass Spectrometry a collection of short biographies on many of the major people who carried out this Encyclopedia of Analytical Science, 2019-04-02 The third edition of the Encyclopedia of Analytical Science Ten Volume Set is a definitive collection of articles covering the latest technologies in application areas such as medicine environmental science food science and geology Meticulously organized clearly written and fully interdisciplinary the Encyclopedia of Analytical Science Ten Volume Set provides foundational knowledge across the scope of modern analytical chemistry linking fundamental topics with the latest methodologies Articles will cover three broad areas analytical techniques e q mass spectrometry liquid chromatography atomic spectrometry areas of application e q forensic environmental and clinical and analytes e g arsenic nucleic acids and polycyclic aromatic hydrocarbons providing a one stop resource for analytical scientists Offers readers a one stop resource with access to information across the entire scope of modern analytical science Presents articles split into three broad areas analytical techniques areas of application and and analytes creating an ideal resource for students researchers and professionals Provides concise and accessible information that is ideal for non specialists and readers from undergraduate levels and higher **Encyclopedia of Spectroscopy and** Spectrometry, 2016-09-22 This third edition of the Encyclopedia of Spectroscopy and Spectrometry Three Volume Set provides authoritative and comprehensive coverage of all aspects of spectroscopy and closely related subjects that use the same fundamental principles including mass spectrometry imaging techniques and applications It includes the history theoretical background details of instrumentation and technology and current applications of the key areas of spectroscopy The new edition will include over 80 new articles across the field These will complement those from the previous edition which have been brought up to date to reflect the latest trends in the field Coverage in the third edition includes Atomic spectroscopy Electronic spectroscopy Fundamentals in spectroscopy High Energy spectroscopy Magnetic resonance Mass spectrometry Spatially resolved spectroscopic analysis Vibrational rotational and Raman spectroscopies The new edition is aimed at professional scientists seeking to familiarize themselves with particular topics quickly and easily This major reference work continues to be clear and accessible and focus on the fundamental principles techniques and applications of spectroscopy and spectrometry Incorporates more than 150 color figures 5 000 references and 300 articles for a thorough examination of the field Highlights new research and promotes innovation in applied areas ranging from food science and forensics to biomedicine and health Presents a one stop resource for quick access to answers and an in depth examination of topics in the spectroscopy and spectrometry arenas Principles of Mass Spectrometry Applied to Biomolecules Chava

Lifshitz, Julia Laskin, 2006-11-02 An extensive compilation of articles by leading professionals this reference explains the fundamental principles of mass spectrometry as they relate to the life sciences Topics covered include spectroscopy energetics and mechanisms of peptide fragmentation electron capture dissociation ion ion and ion molecule reactions reaction dynamics collisional activation soft landing protein structure and interactions thermochemistry and more The book empowers readers to develop new ways of using these techniques Handbook on the Physics and Chemistry of Rare Earths, 2014-07-10 The Handbook on the Physics and Chemistry of Rare Earths is an ongoing series covering all aspects of rare earth science chemistry life sciences materials science and physics The main emphasis of the Handbook is on rare earth elements Sc Y and the lanthanides La through Lu but information is also included whenever relevant on the closely related actinide elements. The individual chapters are comprehensive broad up to date critical reviews written by highly experienced invited experts The series which was started in 1978 by Professor Karl A Gschneidner Jr combines and integrates both the fundamentals and applications of these elements and now publishes two volumes a year Individual chapters are comprehensive broad critical reviews Contributions are written by highly experienced invited experts Up to date overviews of developments in the field The Encyclopedia of Mass Spectrometry Michael L. Gross, Richard Caprioli, 2003 Presents information on the biographies of recognized pioneers and innovators in the field of mass spectrometry Highlights over 120 innovators in mass spectrometry including several Nobel Prize winners Discusses instrumentation and their uses also providing interesting information on the careers characters and life stories of the people who did the work Offers unique insight into the careers and personalities of luminaries in the field **Encyclopedia of Chemical Physics and Physical Chemistry** John H. Moore, Nicholas D. Spencer, 2023-07-03 The Encyclopedia of Physical Chemistry and Chemical Physics introduces possibly unfamiliar areas explains important experimental and computational techniques and describes modern endeavors The encyclopedia quickly provides the basics defines the scope of each subdiscipline and indicates where to go for a more complete and detailed explanation Particular attention has been paid to symbols and abbreviations to make this a user friendly encyclopedia Care has been taken to ensure that the reading level is suitable for the trained chemist or physicist The encyclopedia is divided in three major sections FUNDAMENTALS the mechanics of atoms and molecules and their interactions the macroscopic and statistical description of systems at equilibrium and the basic ways of treating reacting systems. The contributions in this section assume a somewhat less sophisticated audience than the two subsequent sections At least a portion of each article inevitably covers material that might also be found in a modern undergraduate physical chemistry text METHODS the instrumentation and fundamental theory employed in the major spectroscopic techniques the experimental means for characterizing materials the instrumentation and basic theory employed in the study of chemical kinetics and the computational techniques used to predict the static and dynamic properties of materials APPLICATIONS specific topics of current interest and intensive research For the practicing physicist or chemist this

encyclopedia is the place to start when confronted with a new problem or when the techniques of an unfamiliar area might be exploited For a graduate student in chemistry or physics the encyclopedia gives a synopsis of the basics and an overview of the range of activities in which physical principles are applied to chemical problems It will lead any of these groups to the salient points of a new field as rapidly as possible and gives pointers as to where to read about the topic in more detail

Theory and Applications of Computational Chemistry Clifford Dykstra, Gernot Frenking, Kwang Kim, Gustavo Scuseria, 2011-10-13 Computational chemistry is a means of applying theoretical ideas using computers and a set of techniques for investigating chemical problems within which common questions vary from molecular geometry to the physical properties of substances Theory and Applications of Computational Chemistry The First Forty Years is a collection of articles on the emergence of computational chemistry. It shows the enormous breadth of theoretical and computational chemistry today and establishes how theory and computation have become increasingly linked as methodologies and technologies have advanced Written by the pioneers in the field the book presents historical perspectives and insights into the subject and addresses new and current methods as well as problems and applications in theoretical and computational chemistry Easy to read and packed with personal insights technical and classical information this book provides the perfect introduction for graduate students beginning research in this area It also provides very readable and useful reviews for theoretical chemists Written by well known leading experts Combines history personal accounts and theory to explain much of the field of theoretical and computational chemistry Is the perfect introduction to the field The Encyclopedia of Mass **Spectrometry, Ten-Volume Set**, 2013-09-27 Overview The Encyclopedia of Mass Spectrometry The need for an encyclopedia of mass spectrometry MS becomes apparent when considering the subject s evolution By 1990 MS had evolved as a discipline and as a technique for solving problems in chemistry Along with nuclear magnetic resonance and optical spectroscopy it was a tool for compound identification For complex mixtures as found in environmental chemistry flavors energy materials and small molecule metabolism gas chromatography mass spectrometry had become the premier analytical method Despite these advances MS played in 1990 only a small role in polar and large molecule analysis Field desorption fast atom bombardment and Cf 252 plasma desorption gently pushed it into peptide sequencing and molecular weight determination of larger polymers Although these ionizations had limitations when they were coupled with tandem mass spectrometers the future became clearer MS now awaited the development of new ionization methods that would extend its capabilities into many different research laboratories The inventions of electrospray ionization ESI and matrix assisted laser desorption ionization MALDI in the late 1980s opened the door for that greater role Even the discipline of MS could expand by embracing the chemical physical studies of proteins and oligodeoxynucleotides in the gas phase The broad applicability of MS to a multitude of chemical physical and biological problems makes it now the central tool in chemical analysis No longer a specialist s tool it has assumed broad applicability and availability To permit a full and fruitful expansion in other

disciplines the Encyclopedia of Mass Spectrometry is designed to be a learning tool to newcomers who do not have the theoretical and practical background needed to take advantage of the possibilities of MS Moreover the field is now so broad that the specialist also needs a resource to allow exploration of its vast reaches The encyclopedia meets that need and strives to be an entrance into the subject and to serve as its major reference work Volume 1 Theory and Ion Chemistry Volume 1 begins with two theory chapters The first discusses theoretical aspects of ion collisions chemistry and dynamics and the second introduces ab initio calculations of ions The latter has become a nearly indispensable tool in ion chemistry studies today Instrumentation is essential in fundamental investigations Chapter 3 introduces instrumentation with an emphasis on unusual instrumentation generally not commercially available Ion traps ion cyclotron resonance mass spectrometers and time of flight instruments which are important in both fundamental studies and in applications are also covered Chapter 4 discusses myriad means of performing spectroscopic experiments on ions In the next chapter various methods of measuring thermodynamic information about ions are introduced and evaluated Collisional activation and dissociation processes in various incarnations are in Chapter 6 Mobility experiments are the focus of the next chapter which covers fundamental aspects and applications of this rapidly growing technology Various means and uses of changing charge states of ions is the topic of chapter 8 Chapters 9 and 10 introduce the ion chemistry of organic ions positive and negative respectively The last three chapters Chapter 11 13 are expositions of the ion chemistry of clusters and solvation phenomena inorganic chemistry and the rapidly expanding area of biochemistry Volume 2 Biological Applications Part A The focus of Volume 2 is peptides and proteins The organization emphasizes separation techniques preparation protocols and fundamentals of ionic gas phase species of biological importance This volume is divided into four sections 1 experimental approaches and protocols 2 sequence analysis 3 other structural analyses and 4 targeted applications. The first section encompass separation procedures e g 2 D gel electrophoresis sample preparation e g desalting and enzyme digestion and instrumentation issues e g high resolving power molecular weight determination protein chips and quantification H D exchange analysis of membrane proteins and bioinformatics are included The next section on sequencing covers high energy and low energy CAD protein identification fundamentals of peptide fragmentation bottom up and top down strategies chemical derivatization and post source decay with MALDI A section on structure analysis includes primary structure determination and issues with studying quaternary structure protein protein and protein ligand complexes disulfide analysis phosphopeptides and phosphoproteins selenoproteins nitrated proteins metal ion binding and oxidized proteins Additional coverage of methods for studying the biophysics of proteins is provided in Volume 6 The last chapter Targeted Applications focuses on neuropeptides clinical applications enzyme kinetics imaging and single cell analysis Volume 3 Biological Applications Part B Over the past decades enormous gains have been made towards the analysis of all the biomolecules in cells Although early attention was focused on peptides and proteins a wealth of information is arising about other major biomolecules including nucleic acids lipids and

carbohydrates In no small way modern ionization methods especially electrospray and matrix assisted laser desorption have provided a quantum leap in the capabilities of the tools we can now deploy in answering biological questions involving structure and molecular weight of virtually every type of molecule in the cell Volume 3 covers classes carbohydrates nucleic acids and lipids In addition special areas of application are also included such as pharmaceuticals natural products isotope ratio methods for biomolecules analysis and clinical applications. The articles are arranged under general headings for continuity and ease of access although several of these are of interest across the various disciplines The articles cover basics and sufficient additional detail to bring the reader up to date on a given subject Some advanced topics are also covered either in a special section of an article or in additional reading citations Volume 4 Organic and Organometallic Compounds This volume presents a cross section of applications in organic and organometallic chemistry in two parts Chapters 1 to 6 are devoted to the fundamentals whereas chapters 7 and 8 cover applications to organic and organometallic compounds either available as pure compounds or present in complex mixtures Chapter 1 describes the theory for organic mass spectrometry building on and complementing material in Volume 1 The themes for Chapter 2 are the structures and properties of gas phase ions of conventional distonic and non covalent complexes Chapter 3 covers methodology used in study of gas phase ions Chapters 4 and 5 turn to mechanisms of both unimolecular and bimolecular reactions of ions and include topics in stereochemistry and radical chemistry Chapter 6 contains a number of articles on the formation and reactivity of metal ion complexes and organometallic cations and anions drawing connections with molecular recognition catalysis and organic synthesis Chapter 7 deals with the structure determination of organic compounds including chiral compounds and natural products In chapter 8 are contributions that provide illustrative examples of the determination of organic compounds present at low levels in complex samples that originate from various natural and biological sources Included is an article on the determination of explosives Volume 5 Elemental and Isotope Ratio Mass Spectrometry This volume focuses on 1 the plethora of mostly atomic ionization techniques that have been coupled to MS for elemental analysis the measurement of isotope ratios and even the determination of inorganic compounds and 2 the precise measurement of isotope ratios of organic elements as small gas molecules by isotope ratio mass spectrometry IRMS Volume 6 Ionization Methods Volume 6 captures the story of molecular ionization and its phenomenal evolution that makes mass spectrometry the powerful method it is today Chapters 1 and 2 cover fundamentals and various issues that are common to all ionization e g accurate mass isotope clusters and derivatization Chapters 3 9 acknowledge that some ionization methods are appropriate for gas phase molecules and others for molecules that are in the solid or liquid states Chapters 3 6 cover gas phase molecules dividing the subject into 1 ionization of gas phase molecules by particles e g EI 2 ionization by photons 3 ionization by ion molecule and molecule molecule reactions e g APCI and DART and ionization in Strong electric fields i e Electrohydrodynamic and Field Ionization Desorption Ionization in a Strong Electric Field illustrates the transition to ionization of molecules in the solid or liquid states

covered in Chapters 7 9 1 spray methods for ionization e g electrospray 2 desorption ionization by particle bombardment e g FAB and 3 desorption by photons e g MALDI Electrospray and MALDI also lead to applications in biophysical chemistry the theme of Chapter 10 Chapter 11 reconsiders ionization from the view of choosing an ionization method The range of subjects is from ionization of organic and biomolecules to the study of microorganisms Volume 7 Mass Analyzers The volume is under preparation Volume 8 Hyphenated Methods Starting with gas chromatography mass spectrometry GC MS and continuing through GCxGC MS LC MSn and LC NMR MS hyphenated methods have revolutionized chemical analysis This volume covers that revolution in two parts The first Chapters 1 4 describes principles instrumentation and technology and the second Chapters 5 10 organizes major application areas in GC MS and LC MS After a general introduction Chapter 1 attention is paid to principles and instrumentation of GC MS Chapter 2 and LC MS Chapter 3 Other hyphenated methods including online combinations of capillary electromigration methods and supercritical fluid chromatography with mass spectrometry are in Chapter 4 Applications are then covered in the remaining chapters. The application oriented chapters are focused on the role of mainly LC MS in the pharmaceutical field Chapter 5 and biochemical and biotechnological applications Chapter 10 and the application of both GC MS and LC MS in relation to environmental analysis Chapter 6 food safety and food analysis Chapter 7 characterization of natural products Chapter 8 and clinical toxicological and forensic analysis Chapter 9 Volume 9 History of Mass Spectrometry This volume is under preparation Volume 10 Index This multi volume work is the first to provide unparalleled and comprehensive coverage of the full range of topics and techniques Suitable for new graduate students who are interested but not yet versed in the subject of mass spectrometry Techniques methods and applications of mass spectrometry are described in considerable detail including limitations current problems and areas in which the method does not succeed well Enzyme Inhibition in Drug Discovery and Development Chuang Lu, Albert P. Li, 2010-01-26 The science and applied approaches of enzyme inhibition in drug discovery and development Offering a unique approach that includes both the pharmacologic and pharmaco kinetic aspects of enzyme inhibition Enzyme Inhibition in Drug Discovery and Development examines the scientific concepts and experimental approaches related to enzyme inhibition as applied in drug discovery and drug development With chapters written by over fifty leading experts in their fields Enzyme Inhibition in Drug Discovery and Development fosters a cross fertilization of pharmacology drug metabolism pharmacokinetics and toxicology by understanding the good inhibitions desirable pharmacological effects and bad inhibitions drug drug interactions and toxicity The book discusses The drug discovery process including drug discovery strategy medicinal chemistry analytical chemistry drug metabolism pharmacokinetics and safety biomarker assessment The manipulations of drug metabolizing enzymes and transporters as well as the negative consequences such as drug drug interactions The inhibition of several major drug target pathways such as the GPCR pathway the NFkB pathway and the ion channel pathway Through this focused single source reference on the fundamentals of drug discovery and development researchers in drug metabolism and

pharmacokinetics DMPK will learn and appreciate target biology in drug discovery discovery biologists and medicinal chemists will also broaden their understanding of DMPK The Chemistry of the Actinide and Transactinide Elements (Set Vol.1-6) L.R. Morss, Norman M. Edelstein, Jean Fuger, 2010-10-21 The fourth edition of The Chemistry of the Actinide and Transactinide Elements comprises all chapters in volumes 1 through 5 of the third edition published in 2006 plus a new volume 6 To remain consistent with the plan of the first edition to provide a comprehensive and uniform treatment of the chemistry of the actinide and transactinide elements for both the nuclear technologist and the inorganic and physical chemist and to be consistent with the maturity of the field the fourth edition is organized in three parts The first group of chapters follows the format of the first and second editions with chapters on individual elements or groups of elements that describe and interpret their chemical properties A chapter on the chemical properties of the transactinide elements follows The second group chapters 15 26 summarizes and correlates physical and chemical properties that are in general unique to the actinide elements because most of these elements contain partially filled shells of 5f electrons whether present as isolated atoms or ions as metals as compounds or as ions in solution The third group chapters 27 39 focuses on specialized topics that encompass contemporary fields related to actinides in the environment in the human body and in storage or wastes Two appendices at the end of volume 5 tabulate important nuclear properties of all actinide and transactinide isotopes Volume 6 Chapters 32 through 39 consists of new chapters that focus on actinide species in the environment actinide waste forms nuclear fuels analytical chemistry of plutonium actinide chalcogenide and hydrothermal synthesis of actinide compounds The subject and author indices and list of contributors encompass all six volumes The Encyclopedia of Mass Spectrometry Richard Caprioli, 2005-11-11 Volume 3 looks at classes of biomolecules including carbohydrates nucleic acids and lipids In addition special areas of application are included such as pharmaceuticals natural products isotope ratio methods for biomolecules analysis and clinical applications The articles are arranged under general headings for continuity and ease of access although several of these are of interest across the various disciplines. The articles are intended to teach and therefore strive to cover basics and sufficient additional detail to bring the reader up to date on a given subject Some advanced topics are also covered either in a special section of articles or in additional reading citations Gas-Phase IR Spectroscopy and Structure of Biological Molecules Anouk M. Rijs, Jos Oomens, 2015-06-03 The series Topics in Current Chemistry presents critical reviews of the present and future trends in modern chemical research. The scope of coverage is all areas of chemical science including the interfaces with related disciplines such as biology medicine and materials science The goal of each thematic volume is to give the non specialist reader whether in academia or industry a comprehensive insight into an area where new research is emerging which is of interest to a larger scientific audience Each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole The most significant developments of the last 5 to 10 years are presented using selected examples to illustrate the principles discussed The coverage is not

intended to be an exhaustive summary of the field or include large quantities of data but should rather be conceptual concentrating on the methodological thinking that will allow the non specialist reader to understand the information presented Contributions also offer an outlook on potential future developments in the field Review articles for the individual volumes are invited by the volume editors Readership research chemists at universities or in industry graduate students

Natural Products Analysis Vladimir Havlicek, Jaroslav Spizek, 2014-09-17 This book highlights analytical chemistry instrumentation and practices applied to the analysis of natural products and their complex mixtures describing techniques for isolating and characterizing natural products Applies analytical techniques to natural products research an area of critical importance to drug discovery Offers a one stop shop for most analytical methods x ray diffraction NMR analysis mass spectrometry and chemical genetics Includes coverage of natural products basics and highlights antibacterial research particularly important as efforts to combat drug resistance gain prominence Covers instrumental techniques with enough detail for both current practitioners and beginning researchers Organic Trace Analysis Reinhard Nießner, Andreas Schäffer, 2024-09-23 Organic contaminants even in very low concentrations can have toxic and ecotoxic effects on exposed organisms Detection and quantification of such trace amounts in diverging matrices e g water air soil food tissue organisms is challenging and great carefulness and strategic thinking is needed to get reliable results along the way from taking samples up to the final analysis In the 2nd edition besides revisions of existing chapters new analytical technologies and recent application examples are presented non target mass spectrometric analysis trace analysis of per and polyfluoroalkylated forever chemicals organophosphorus esters nerve agents and micro and nanoplastic particles in the environment Students will learn about peculiarities and state of the art organic trace analysis and acquire basic and advanced principles of statistical evaluation of analytical results quality control strategies and good laboratory practices sampling techniques from various matrices sample treatment enrichment and clean up techniques chromatographic analyses including hyphenated techniques and spectroscopy as well mass spectrometry and bioanalytical tools An extended chapter on selected applications will transfer the theoretical understanding into applied scientific problems Students will profit from a comprehensive and state of the art overview of organic trace analyses and from an extensive collection of relevant literature

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