

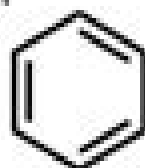
Summary: Anti-Aromaticity

Aromatic

*unusually
stable*

- Cyclic
- Conjugated
- $(4n+2)$ Pi electrons
- Flat

e.g.



benzene

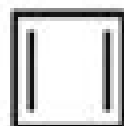
(resonance
energy of 36 kcal/mol)

Anti-Aromatic

*unusually
unstable*

- Cyclic
- Conjugated
- $(4n)$ Pi electrons
- Flat

e.g.



cyclobutadiene

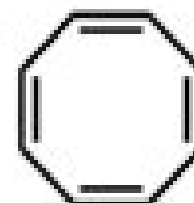
(only stable below
 $-100\text{ }^{\circ}\text{C}$)

Non-Aromatic

everything else

*Fails any one
of the 4 criteria
on the left*

e.g.



cyclooctatetraene

(adopts a tub-like
shape to "escape"
anti-aromaticity)

Aromaticity And Antiaromaticity

Errol G. Lewars



Aromaticity And Antiaromaticity:

Aromaticity and Antiaromaticity Miquel Solà, Alexander I. Boldyrev, Michal K. Cyrański, Tadeusz M. Krygowski, Gabriel Merino, 2022-10-10 Aromaticity and Antiaromaticity A comprehensive review of the science of aromaticity as well as its evolution from benzene to atomic clusters In Aromaticity and Antiaromaticity Concepts and Applications a team of accomplished chemists delivers a comprehensive exploration of the evolution and critical aspects of aromaticity The book examines the new global criteria used to evaluate aromaticity including the Nucleus Independent Chemical Shift NICS index and the electronic indices based on electronic properties Additional discussions of inorganic aromatic compounds developed in this century which give rise to new concepts like multifold aromaticity are included Three dimensional aromaticity found in fullerenes and nanotubes M bius aromaticity present in some annulenes and excited state aromaticity are explored as well This volume explores the geometrical electronic magnetic and thermodynamic characteristics of aromatic and antiaromatic compounds and their reactivity properties It also provides A thorough historical overview of aromaticity as well as simple electronic and structural models Comprehensive explorations of organic and inorganic aromatic compounds concepts of stability and reactivity and geometric energetic magnetic and electronic criteria of descriptors of aromaticity Practical discussions of heteroaromaticity as well as M bius aromaticity and excited state aromaticity In depth examinations of sigma pi delta and phi aromaticity Perfect for graduate students researchers and academics interested in aromaticity organometallic chemistry and computational chemistry Aromaticity and Antiaromaticity Concepts and Applications will also earn a place in the libraries of professionals and researchers working in organic inorganic and physical chemistry

Aromaticity and Antiaromaticity Vladimir I. Minkin, Mikhail Nikolaevich Glukhovtsev, Mikhail N. Glukhovtsev, Boris I. A. Kovlevich Simkin, 1994-04-14 Designed to assist chemists in integrating the results of calculations on molecules and ions into their general body of chemical knowledge Contains recent contributions from theoretical and computational chemistry to the development of the concept of aromaticity antiaromaticity and its expansion into new areas such as organometallic and cluster compounds and three dimensional structures Updates the modern status of aromaticity and covers basic principles and experimental applications "Aromaticity, Pseudo-aromaticity, Anti-aromaticity" Ernst David Bergmann, Bernard Pullman, 1971

Nanoclusters Purusottam Jena, Albert Welford Castleman, 2011-02-08 This comprehensive book on Nanoclusters comprises sixteen authoritative chapters written by leading researchers in the field It provides insight into topics that are currently at the cutting edge of cluster science with the main focus on metal and metal compound systems that are of particular interest in materials science and also on aspects related to biology and medicine While there are numerous books on clusters the focus on clusters as a bridge across disciplines sets this book apart from others Delivers cutting edge coverage of cluster science Covers a broad range of topics in physics chemistry and materials science Written by leading researchers in the field

Chemical Reactivity Theory Pratim Kumar Chattaraj, 2009-02-23 In the 1970s

Density Functional Theory DFT was borrowed from physics and adapted to chemistry by a handful of visionaries Now chemical DFT is a diverse and rapidly growing field its progress fueled by numerous developing practical descriptors that make DFT as useful as it is vast With 34 chapters written by 65 eminent scientists from 13 different countries **Metal-Metal Bonding** Gerard Parkin, 2010-03-04 None *Aromaticity and Metal Clusters* Pratim Kumar Chattaraj, 2010-10-15 Metal clusters are an intermediate state between molecules and the extended solid show peculiar bonding and reactivity patterns Their significance is critical to many areas including air pollution interstellar matter clay minerals photocatalysis quantum dots and virus crystals In *Aromaticity and Metal Clusters* dozens of international experts explore not only the basic aspects of aromaticity but also the structures properties reactivity stability and other consequences of the aromaticity of a variety of metal clusters Although the concept of aromaticity has been known for nearly two centuries there is no way to measure it experimentally and no theoretical formula to calculate it In order to gain insight into its exact nature the authors of this volume examine various indirect characteristics such as geometrical electronic magnetic thermodynamic and reactivity considerations The book begins by discussing the evolution of aromaticity from benzene to atomic clusters Next more specialized chapters focus on areas of significant interest Topics discussed include Computational studies on molecules with unusual aromaticity Electronic shells and magnetism in small metal clusters A density functional investigation on the structures energetics and properties of sodium clusters through electrostatic guidelines and molecular tailoring The correlation between electron delocalization and ring currents in all metallic aromatic compounds Phenomenological shell model and aromaticity in metal clusters Rationalizing the aromaticity indexes used to describe the aromatic behavior of metal clusters 5f orbital successive aromatic and antiaromatic zones in triangular uranium cluster chemistry This collection of diverse contributions composed of the work of scientists worldwide is destined to not only answer puzzling questions about the nature of aromaticity but also to provoke further inquiry in the minds of researchers *Computational Inorganic and Bioinorganic Chemistry* Edward I. Solomon, Robert A. Scott, R. Bruce King, 2013-02-19 Over the past several decades there have been major advances in our ability to computationally evaluate the electronic structure of inorganic molecules particularly transition metal systems This advancement is due to the Moore's Law increase in computing power as well as the impact of density functional theory DFT and its implementation in commercial and freeware programs for quantum chemical calculations Improved pure and hybrid density functionals are allowing DFT calculations with accuracy comparable to high level Hartree Fock treatments and the results of these calculations can now be evaluated by experiment When calculations are correlated to and supported by experimental data they can provide fundamental insight into electronic structure and its contributions to physical properties and chemical reactivity This interplay continues to expand and contributes to both improved value of experimental results and improved accuracy of computational predictions The purpose of this EIC Book is to provide state of the art presentations of quantum mechanical and related methods and their applications written by many

of the leaders in the field Part 1 of this volume focuses on methods their background and implementation and their use in describing bonding properties energies transition states and spectroscopic features Part 2 focuses on applications in bioinorganic chemistry and Part 3 discusses inorganic chemistry where electronic structure calculations have already had a major impact This addition to the EIC Book series is of significant value to both experimentalists and theoreticians and we anticipate that it will stimulate both further development of the methodology and its applications in the many interdisciplinary fields that comprise modern inorganic and bioinorganic chemistry This volume is also available as part of Encyclopedia of Inorganic Chemistry 5 Volume Set This set combines all volumes published as EIC Books from 2007 to 2010 representing areas of key developments in the field of inorganic chemistry published in the Encyclopedia of Inorganic Chemistry Find out more at <http://eu.wiley.com/WileyCDA/WileyTitle/productCd/1119994284.html>

Organophosphorus Chemistry 2018 György Keglevich, 2020-03-05 Organophosphorus chemistry is an important discipline within organic chemistry Phosphorus compounds such as phosphines trialkyl phosphites phosphine oxides chalcogenides phosphonates phosphinates and P O H species etc may be important starting materials or intermediates in syntheses Let us mention the Wittig reaction and the related transformations the Arbuzov and the Pudovik reactions the Kabachnik Fields condensation the Hirao reaction the Mitsunobu reaction etc Other reactions e g homogeneous catalytic transformations or C C coupling reactions involve P ligands in transition metal Pt Pd etc complex catalysts The synthesis of chiral organophosphorus compounds means a continuous challenge Methods have been elaborated for the resolution of tertiary phosphine oxides and for stereoselective organophosphorus transformations P heterocyclic compounds including aromatic and bridged derivatives P functionalized macrocycles dendrimers and low coordinated P fragments are also of interest An important segment of organophosphorus chemistry is the pool of biologically active compounds that are searched and used as drugs or as plant protecting agents The natural analogue of P compounds may also be mentioned Many new phosphine oxides phosphinates phosphonates and phosphoric esters have been described which may find application on a broad scale Phase transfer catalysis ionic liquids and detergents also have connections to phosphorus chemistry Green chemical aspects of organophosphorus chemistry e g microwave assisted syntheses solvent free accomplishments optimizations and atom efficient syntheses represent a dynamically developing field Last but not least theoretical approaches and computational chemistry are also a strong sub discipline within organophosphorus chemistry

[Comprehensive Inorganic Chemistry II](#), 2013-07-23 Comprehensive Inorganic Chemistry II Nine Volume Set reviews and examines topics of relevance to today's inorganic chemists Covering more interdisciplinary and high impact areas Comprehensive Inorganic Chemistry II includes biological inorganic chemistry solid state chemistry materials chemistry and nanoscience The work is designed to follow on with a different viewpoint and format from our 1973 work Comprehensive Inorganic Chemistry edited by Bailar Emel us Nyholm and Trotman Dickenson which has received over 2 000 citations The new work will also complement other recent

Elsevier works in this area Comprehensive Coordination Chemistry and Comprehensive Organometallic Chemistry to form a trio of works covering the whole of modern inorganic chemistry Chapters are designed to provide a valuable long standing scientific resource for both advanced students new to an area and researchers who need further background or answers to a particular problem on the elements their compounds or applications Chapters are written by teams of leading experts under the guidance of the Volume Editors and the Editors in Chief The articles are written at a level that allows undergraduate students to understand the material while providing active researchers with a ready reference resource for information in the field The chapters will not provide basic data on the elements which is available from many sources and the original work but instead concentrate on applications of the elements and their compounds Provides a comprehensive review which serves to put many advances in perspective and allows the reader to make connections to related fields such as biological inorganic chemistry materials chemistry solid state chemistry and nanoscience Inorganic chemistry is rapidly developing which brings about the need for a reference resource such as this that summarise recent developments and simultaneously provide background information Forms the new definitive source for researchers interested in elements and their applications completely replacing the highly cited first edition which published in 1973 *The Chemical Bond* Gernot Frenking, Sason Shaik, 2014-07-08 A unique overview of the different kinds of chemical bonds that can be found in the periodic table from the main group elements to transition elements lanthanides and actinides It takes into account the many developments that have taken place in the field over the past few decades due to the rapid advances in quantum chemical models and faster computers This is the perfect complement to Chemical Bonding Fundamentals and Models by the same editors who are two of the top scientists working on this topic each with extensive experience and important connections within the community

Coordination Chemistry of Silicon Prof. Dr. Shigeyoshi Inoue, 2019-03-04 The chemistry of silicon has always been a field of major concern due to its proximity to carbon on the periodic table From the molecular chemist's viewpoint one of the most interesting differences between carbon and silicon is their divergent coordination behavior In fact silicon is prone to form hyper coordinate organosilicon complexes and as conveyed by reports in the literature highly sophisticated ligand systems are required to furnish low coordinate organosilicon complexes Tremendous progress in experimental as well as computational techniques has granted synthetic access to a broad range of coordination numbers for silicon and the scientific endeavor which was ongoing for decades was rewarded with landmark discoveries in the field of organosilicon chemistry Molecular congeners of silicon 0 as well as silicon oxides were unveiled and the prominent group 14 metalloid proved its applicability in homogenous catalysis as a supportive ligand or even as a center of catalytic activity This book focuses on the most recent advances in the coordination chemistry of silicon with transition metals as well as main group elements including the stabilization of low valent silicon species through the coordination of electron donor ligands Therefore this book is associated with the development of novel synthetic methodologies structural elucidations bonding analysis and also possible

applications in catalysis or chemical transformations using related organosilicon compounds **Advances in Heterocyclic Chemistry**, 1993-04-20 Advances in Heterocyclic Chemistry **Aromaticity** Peter Joseph Garratt, 1971 For students in the final year of their chemistry Honours BSc and also to those beginning postgraduate work **Computational Chemistry** Errol G. Lewars, 2010-11-10 This corrected second edition contains new material which includes solvent effects the treatment of singlet diradicals and the fundamentals of computational chemistry Computational Chemistry Introduction to the Theory and Applications of Molecular and Quantum Mechanics is an invaluable tool for teaching and researchers alike The book provides an overview of the field explains the basic underlying theory at a meaningful level that is not beyond beginners and it gives numerous comparisons of different methods with one another and with experiment The following concepts are illustrated and their possibilities and limitations are given potential energy surfaces simple and extended Hückel methods ab initio AM1 and related semiempirical methods density functional theory DFT Topics are placed in a historical context adding interest to them and removing much of their apparently arbitrary aspect The large number of references to all significant topics mentioned should make this book useful not only to undergraduates but also to graduate students and academic and industrial researchers European Journal of Organic Chemistry, 2007 *Aromaticity* Israel Fernandez, 2021-05-16 Evaluating the aromaticity of a molecular system and the influence of this concept on its properties is a crucial step in the development of novel aromatic systems Modern computational methods can provide researchers with a high level of insight into such aromaticity but identifying the most appropriate method for assessing a specific system can prove difficult Aromaticity Modern Computational Methods and Applications reviews the latest state of the art computational methods in this field and discusses their applicability for evaluating the aromaticity of a system In addition to covering aromaticity for typical organic molecules this volume also explores systems possessing transition metals in their structures macrocycles and even transition structures The influence of the aromaticity on the properties of these species including the structure magnetic properties and reactivity is highlighted along with potential applications in fields including materials science and medicinal chemistry Finally the controversial and fuzzy nature of aromaticity as a concept is discussed providing the basis for an updated and more comprehensive definition of this concept Drawing on the knowledge of an international team of experts Aromaticity Modern Computational Methods and Applications is a unique guide for anyone researching studying or applying principles of aromaticity in their work from computational and organic chemists to pharmaceutical and materials scientists Reviews a range of computational methods to assess the aromatic nature of different compounds helping readers select the most useful tool for the system they are studying Presents a complete guide to the key concepts and fundamental principles of aromaticity Provides guidance on identifying which variables should be modified to tune the properties of an aromatic system for different potential applications **Aromatic Hydrocarbons—Advances in Research and Treatment: 2013 Edition**, 2013-06-21 Aromatic Hydrocarbons Advances in Research and Treatment 2013 Edition is a

ScholarlyEditions book that delivers timely authoritative and comprehensive information about Benzene The editors have built Aromatic Hydrocarbons Advances in Research and Treatment 2013 Edition on the vast information databases of ScholarlyNews You can expect the information about Benzene in this book to be deeper than what you can access anywhere else as well as consistently reliable authoritative informed and relevant The content of Aromatic Hydrocarbons Advances in Research and Treatment 2013 Edition has been produced by the world s leading scientists engineers analysts research institutions and companies All of the content is from peer reviewed sources and all of it is written assembled and edited by the editors at ScholarlyEditions and available exclusively from us You now have a source you can cite with authority confidence and credibility More information is available at <http://www.ScholarlyEditions.com> **Progress in Quantum**

Chemistry Research Erik O. Hoffman, 2007 This book presents new and important research from around the world in quantum chemistry which is a branch of theoretical chemistry Quantum chemistry applies quantum mechanics and quantum field theory to address issues and problems in chemistry The description of the electronic behaviour of atoms and molecules as pertaining to their reactivity is one of the applications of quantum chemistry Quantum chemistry lies on the border between chemistry and physics and significant contributions have been made by scientists from both fields It has a strong and active overlap with the field of atomic physics and molecular physics as well as physical chemistry **March's**

Advanced Organic Chemistry Michael B. Smith, 2025-08-25 Leading reference on the theories of organic chemistry now updated to reflect the most recent literature from 2018 to 2023 Building on the success of the 8th Edition as winner of the Textbook Academic Authors Association 2021 McGuffey Longevity Award the revised and updated 9th Edition of March s Advanced Organic Chemistry explains the theories of organic chemistry covers new advances in areas of organic chemistry published between 2018 and 2023 and guides readers to plan and execute multi step synthetic reactions Detailed examples and descriptions of all reactions are included throughout the text As in previous editions the goal of this edition is to give equal weight to three fundamental aspects of the study of organic chemistry reactions mechanisms and structure Specific but specialized areas of organic chemistry such as terpenes polymerization and steroids have been incorporated into primary sections rather than segregated into their own sections The first nine chapters cover general organic chemistry with theoretical principles The next 10 chapters address reactions and mechanistic discussion Appendix A focuses on literature references and resources More than 4 400 references are included throughout the text March s Advanced Organic Chemistry provides information on Localized and delocalized chemical bonding and bonding weaker than covalent Microwave chemistry use of ultrasound mechanochemistry and reactions done under flow conditions Acids and bases irradiation processes stereochemistry structure of intermediates and ordinary and photochemical reactions Mechanisms and methods of determining carbocations carbanions free radicals carbenes and nitrenes Aliphatic alkenyl and alkynyl substitution additions to carbon carbon and carbon hetero bonds eliminations rearrangements and oxidations and reductions This 9th Edition of

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