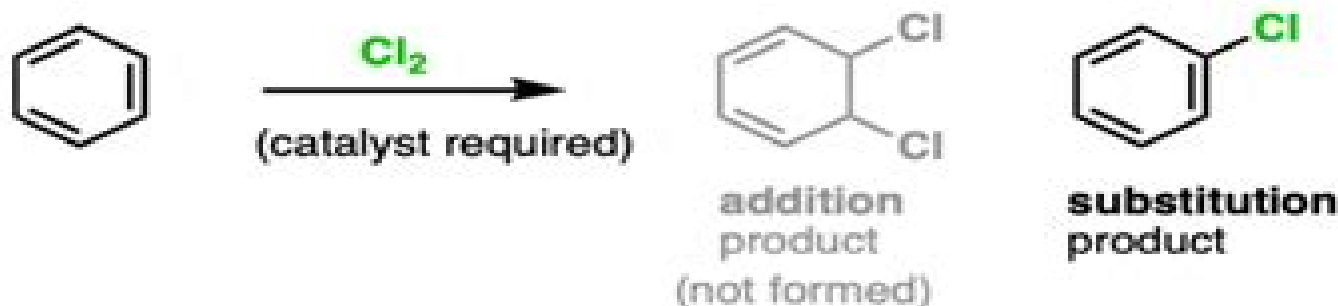


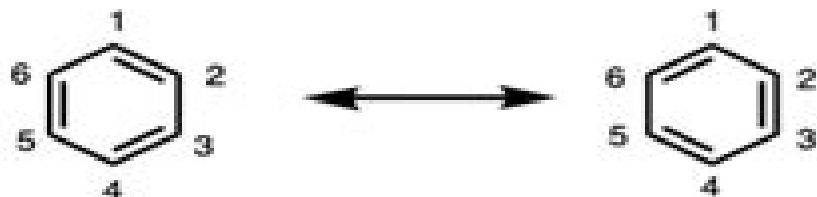
Summary: Aromaticity

Aromaticity is the term given to describe the unusual **stability** of benzene and related molecules. Not related to smells! 😊

- Benzene does not easily undergo **addition** like normal alkenes
- When benzene does undergo reaction, it tends to undergo **substitution** reactions
(and even then, often requires heating and addition of a catalyst)

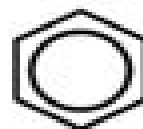


- The measured **resonance energy** of benzene is extremely high (36 kcal/mol) compared to conjugated alkenes like 1,3-cyclohexadiene (2 kcal/mol)
- Unlike dienes, which have alternating bond lengths, **all C-C bond lengths in benzene are identical** (1.40 Å)



Equivalent resonance structures
(not an equilibrium!)

Either structure for benzene is correct
and they can be used interchangeably



Hybrid of these two forms
sometimes drawn like this
to show that the pi-electrons
are "**delocalized**"

- The property of aromaticity is not unique to benzene

Physical Chemistry Of 12dithiole Compounds The Question Of Aromaticity

Israel Fernandez



Physical Chemistry Of 12dithiole Compounds The Question Of Aromaticity:

Whitaker's Books in Print ,1990 **Aromaticity and Antiaromaticity** Miquel Solà,Alexander I. Boldyrev,Michal K. Cyrański,Tadeusz M. Krygowski,Gabriel Merino,2022-10-14 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 *Aromatic Character and Aromaticity* G. M. Badger,1969-01-02 Originally published in 1969 this book analyses the special properties of benzene and its derivatives which give them their distinct aromatic character The text first discusses the structure of benzene including the light shed on it by physical methods and wave mechanics and the structure of polycyclic benzenoid hydrocarbons and heterocyclic aromatic compounds Aromaticity is defined as a function of the electronic structure of the molecule or ion in question and it is shown that this has important consequences in respect of bond lengths resonance energies electronic absorption spectra and induced ring currents Final chapters discuss how far aromatic character and aromaticity are associated with non benzenoid hydrocarbons and with more complex systems **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

Aromaticity and Antiaromaticity Vladimir I. Minkin, Mikhail Nikolaevich Glukhovtsev, Mikhail N. Glukhovtsev, Boris I. 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 Peter J. Garratt, 1986-04-25 Examines aromaticity through the historical and conceptual framework of simple molecular orbital theory This approach is unique in that theoretical considerations are integrated with experimental observations The criteria for aromatic antiaromatic and nonaromatic compounds are discussed in with reference to benzene cyclobutadiene and cyclooctatetraene Also includes a chapter on the likely classes of aromatic compounds

Aromatic Chemistry John D. Hepworth, David R. Waring, Michael J. Waring, 2002 This product is not available separately it is only sold as part of a set There are 750 products in the set and these are all sold as one entity This book provides an up to date and comprehensive account of aromatic chemistry A series of chapters describes the synthesis and reactions of the major functional derivatives of benzene and the more common polycyclic systems The concept of aromaticity and the mechanism of aromatic substitution are discussed as is the use of metals in the synthesis of aromatic compounds Throughout emphasis is placed on mechanisms Worked problems and questions are provided to aid understanding In addition to providing material required by an undergraduate studying chemistry **Aromatic Chemistry** is also ideal for industrial chemists seeking to update their knowledge of this important aspect of chemistry Ideal for the needs of undergraduate chemistry students **Tutorial Chemistry Texts** is a major new series consisting of short single topic or modular texts concentrating on the fundamental areas of chemistry taught in undergraduate science courses Each book provides a concise account of the basic principles underlying a given subject

embodying an independent learning philosophy and including worked examples **Aromatic Chemistry** Malcolm Sainsbury, 1992 All the basic principles of the field of aromatic chemistry are clearly presented in this important account Many compounds of industrial and biological significance are used as examples with consideration given to structure reactions and properties Topics such as thermodynamic versus kinetic control and pericyclic reactions are also introduced In addition to benzene and the classes of aromatic compounds derived from it the text covers polycyclic arenes and the small and large ring systems which are embraced by the wider definition of aromaticity The text will be especially useful for courses in organic chemistry The Structures & Reactions of the Aromatic Compounds Geoffrey Malcolm Badger, 1954 The benzene problem The theoretical solution of the benzene problem and a definition of the term aromatic Some properties of aromatic compounds Addition reactions of aromatic compounds The aromatic double bond The effects of substituents Aromatic substitution reactions The Diels Alder reaction Photo oxidation and photo dimerization Absorption and fluorescence spectra of aromatic compounds Optical activity in aromatic compounds

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