

Four Rules For Aromaticity

Condition #2: Every Atom In The Ring Must Be Conjugated

(alternative): every atom in the ring must have an available p orbital

(alternative): every atom in the ring must be able to participate in resonance



Aromatic

All ring atoms conjugated



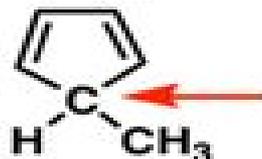
Not aromatic

Nitrogen atom is not conjugated



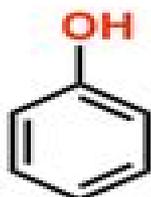
Aromatic

All ring atoms conjugated



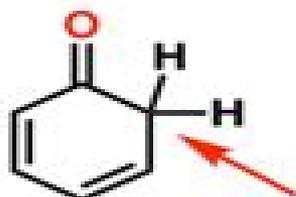
Not aromatic

Carbon is not conjugated (sp^3)



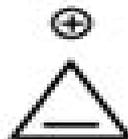
Aromatic

All ring atoms conjugated



Not aromatic

Carbon is not conjugated



Aromatic

All ring atoms conjugated



Not aromatic

Carbon is not conjugated

Key thing to watch out for: an atom attached to four bonds
e.g. sp^3 carbon, or nitrogen

Aromaticity And Other Conjugation Effects

**Vladimir I. Minkin, Mikhail Nikolaevich
Glukhovtsev, Mikhail N.
Glukhovtsev, Boris Iakovlevich Simkin**

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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

Applied Theoretical Organic Chemistry Dean J Tantillo, 2018-03-08 This book provides state of the art information on how studies in applied theoretical organic chemistry are conducted It highlights the many approaches and tools available to those interested in using computational chemistry to predict and rationalize structures and reactivity of organic molecules Chapters not only describe theoretical techniques in detail but also describe recent applications and offer practical advice Authored by many of the world leaders in the field of applied theoretical chemistry this book is perfect for both practitioners of computational chemistry and synthetic and mechanistic organic chemists curious about applying computational techniques to their research Related Link s [Conjugative and inductive interactions in aromatic ketones and](#)

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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

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