

12: Conjugated and Aromatic Molecules

12.1 Conjugated Molecules

1,3-Butadiene (12.1A)

Atomic Orbital Overlap in 1,3-Butadiene

Molecular Orbitals

The Bonding M.O.'s

Conformations

Other Alternating Multiple Bonds

Pentadienes (12.1B)

1,3-Pentadiene

1,4-Pentadiene

1,2-Pentadiene.

Stability of Conjugated Systems (12.1C)

Heats of Hydrogenation of Pentadienes

Heats of Hydrogenation of Butadienes

Aromatic Molecules (12.1D)

12.2 Reactivity of Conjugated Systems

Addition of H-Cl to 1,3-Butadiene (12.2A)

Products

Mechanism

Delocalized Carbocation

Resonance Structures (12.2C)

Carbocation Resonance Structures

Meaning of Resonance Structures

Meaning of The Double Headed Arrow

Other Reactions with Delocalized Intermediates (12.2D)

Acid Catalyzed Hydration

Electrophilic Halogenation

Free Radical Addition of H-Br.

12.3 Writing Resonance Structures

A General Procedure (12.3A)

Carbocations (C⁺) (12.3B)

Carbanions (C⁻) (12.3C)

Radicals (C[•]) (12.3D)

12.4 More on Delocalized Systems

Localized vs. Delocalized Intermediates (12.4A)

Reactions other than Addition (12.4B)

Radical Halogenation

Resonance Forms with Heteroatom

Relative Importance of Resonance Forms

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Benzene (12.5A)

Reactivity

Stability

¹H NMR Spectra

(continued)

The Real Structure of Benzene (12.5B)
 Benzene Geometry
 Benzene Resonance Structures
 Benzene Molecular Orbitals
Benzene MO's, Resonance, and Unusual Properties (12.5C)
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Substituted Benzenes (12.5D)

12.6 Nomenclature of Benzenoid Aromatic Molecules

Monocyclic Arenes (12.6A)
 Systematic Nomenclature
 Common Nomenclature
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 The Phenyl Group
 The Benzyl Group
Polycyclic Arenes (12.6C)

12.7 Aromatic Systems without Benzene Rings

Annulenes (12.7A)
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 Resonance Structures Do Not Tell the Story
MO Diagrams for C₄H₄, C₆H₆ and C₈H₈ (12.7B)
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 Cyclobutadiene.
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 Cyclooctadienyl Dianion

12.8 Making Substituted Benzenes

Electrophilic Aromatic Substitution Mechanism (12.8A)
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 Arenium Ion Formation
 Deprotonation of the Arenium Ion
 Reactions with Substituted Benzenes

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*Formation of the Electrophile (12.8B)**Halogenation**Sulfonation**Nitration.**Alkylation**NH₂ and OH Groups on Arenes (12.8C)**Synthesis of Aniline (Ph-NH₂)**Synthesis of Phenol (Ph-OH)**Acidity of Arene OH Groups**Basicity of Arene NH₂ Groups***12.9 Spectrometry of Conjugated and Aromatic Molecules***NMR Spectral Data (12.9A)**¹H Chemical Shifts**¹³C Chemical Shifts**UV-Visible Spectral Data (12.9B)**Conjugated Polyenes**The Electron Excitation Process**Arenes**The Use of UV-Visible Data**Infrared Spectrometry (12.9C)*