CHAPTER OUTLINES/WORKSHEETS

CHAPTER 15

BENZENE AND AROMATICITY

I. AROMATIC HYDROCARBONS

1. Sources

2. Nomenclature of benzene derivatives
   a. Benzene, toluene, phenol, aniline, acetophenone, benzaldehyde, benzoic acid, benzonitrile, xylene, styrene
   b. Phenyl and benzyl group
   c. Ortho, meta and para
   d. Numbering, alphabetical order

3. Polycyclic Compounds
   a. Naphthalene, anthracene, phenanthrene

II. STRUCTURES

1. Kekulé structure
   a. Number of substitution products
   b. Stability (36 kcals/mole stabilization)

2. Resonance Structures
   a. Pictorial representations

3. Molecular Orbital Description
   a. Three bonding, three antibonding orbitals

4. Hückel [4n + 2] Rule
   a. Planar, monocyclic systems
   b. Cyclobutadiene, benzene, cyclooctatetraene
III. AROMATIC IONS

1. Cations, radicals, and anions
   a. Cyclopentadiene, cycloheptatriene
   b. Resonance structures
   c. Stability and the Hückel rule

2. Heterocycles (pyridine, pyrrole)
   a. Resonance Structures
   b. Stability

IV. NAPHTHALENE

1. Polycyclic aromatic hydrocarbons

V. SPECTROSCOPY

1. IR Spectroscopy (C-H = 3030 and 1600-1450 cm\(^{-1}\))

2. NMR Spectroscopy
   a. Aromatic ring current
   b. Location of chemical shift due to aromatic ring
      Carbon (110-160 ppm — aromatic ring carbons)
      Proton (2.3-3.0 ppm — benzylic/8.0-6.5 ppm — aryl)

Chapter 15 Worksheet

What is a phenyl group? What common abbreviations are used to designate this group?

What is a benzyl group?

How are multiply-substituted benzene rings named?

What are the ortho, para, and meta positions on a substituted benzene ring?
Explain how four different dibrominated products might arise from the dibromination of benzene? The fact that only three are actually found can be explained by what phenomena?

What amount of resonance stabilization does benzene possess? How can this be determined?

Why does this explain the fact that benzene doesn't undergo electrophilic addition reactions as readily as do normal alkenes?

How do the carbon-carbon bond lengths in benzene compare to the lengths of C-C and C=C?

How does Kekulé's structure depiction of benzene differ from that proposed by modern resonance theory?

Draw an energy level diagram for the molecular orbitals of benzene. Which orbitals are degenerate? Which orbitals are bonding? Which are antibonding?

What features are common to aromatic (benzenoid) compounds?

What is the Hückel rule? Is cyclobutadiene aromatic? What about cyclooctatetraene? Why are 4n + 2 electrons in a monocyclic conjugated pi-system so stable?

Why is cyclopentadiene one of the most acidic hydrocarbons known?

Are the cyclopentadienyl radical and cation stabilized in any way?

Why is the cycloheptatrienyl cation extraordinarily stable?

What is a heterocycle?

How does the bonding of nitrogen differ between pyrrole and pyridine?

Why is naphthalene considered to be aromatic?

What is special about the ¹H NMR of aromatic compounds? Why does the ¹H NMR spectrum of [18]-annulene show a resonance upfield of TMS?