2.S: BENZENE AND AROMATICITY (SUMMARY)

CONCEPTS & VOCABULARY

15.0 Introduction

- Aromatic compounds contain ring structures with a special type of resonance delocalization.
- Aromatic compounds can be drawn with alternating single and double bonds, each atom in the ring must have a p-orbital available.

15.1 Naming Aromatic Compounds

- Disubstituted benzene derivatives are often named using ortho (1,2), meta (1,3) and para (1,4).
- There are common benzene derivative names that are used by IUPAC such as toluene, phenol, benzoic acid and benzaldehyde.
- A benzene group that is named as a substituent is called phenyl.
- A benzene with a CH_2 as a substituent group is called benzyl.

15.2 Structure and Stability of Benzene

- Benzene does not undergo the same reactions that alkenes do, due to its aromatic stability.
- Aromatic molecules must have all ring atoms in the same plane to allow delocalization of the pi electrons.
- Heats of hydrogenation can be used to show the special stability of benzene compared to what would be expected for a theoretical cyclohexatriene molecule.

15.3 Aromaticity and the Hückel 4n + 2 Rule

- The four criteria for aromaticity are that the molecule must:
  - be cyclic
  - be planar
  - be fully conjugated
  - have 4n+2 π Electrons
- Ionic molecules and heterocyclic molecules can also be aromatic if they meet the four criteria.

15.4 Aromatic Ions

- Carbanions and carbocations that meet the rules for aromaticity are also aromatic.

15.5 Aromatic Heterocycles: Pyridine and Pyrrole

- Heterocycles that meet the rules for aromaticty are also aromatic.
- If a lone pair of electrons on a ring atom can result in 4n+2 π Electrons, they will be in a p-orbital. If not, they will remain in hybrid orbitals.

15.6 Polycyclic Aromatic Compounds

- Benzene rings can be fused together to give larger aromatic compounds with mutliple rings called polycyclic aromatic compounds (or polycyclic aromatic hydrocarbons).

15.7 Spectroscopy of Aromatic Compounds

- Aromatic compounds can be identified by common infrared absorptions in the 3000-3100 cm^{-1} and 1500-1600 cm^{-1}.
- In ^1H NMR, aromatic hydrogens appear in the 6.5-8 ppm region.

SKILLS TO MASTER

- Skill 15.1 Using IUPAC rules to name substituted benzene molecules.
- Skill 15.2 Use heats of hydrogenation to explain aromatic stabilization.
- Skill 15.3 Draw molecular orbital diagram for benzene (all 6 MO's).
- Skill 15.4 Use the criteria for aromaticity to determine if a molecule is aromatic or not.
- Skill 15.5 Determine whether lone pairs of electrons for ions and heterocycles will be in p orbitals or hybrid orbitals.
- Skill 15.6 Identify aromatic absorbances in infrared spectroscopy.
- Skill 15.7 Identify aromatic resonances in ^1H NMR spectroscopy.