

Aromatic Compounds

Aromatic Compounds

EQ: How are aromatic compounds different from alkanes, alkenes and alkynes?

- Resonance structure
- Aromatic
- Ortho
- Meta
- Para
- Phenyl
- benzyl

- **EQ: Explain the resonance structure for Benzene.**

EQ: What structure for Benzene did Kekule propose?

Structure of Benzene

1. Kekulé proposal (Section 5.1)

Benzene is 1,3,5-cyclohexatriene, and all carbons are equivalent.

Draw cyclohexene and show the products formed when cyclohexene reacts with ...

- KMnO_4 in basic medium
- water (hydration)
- HCl

Benzene does not react with KMnO_4 , H_2O and HCl

EQ: What structure for Benzene did Kekule propose?

Structure of Benzene

1. Kekulé proposal (Section 5.1)

Benzene is 1,3,5 cyclohexatriene, and all carbons are equivalent.

This proposal doesn't account for the stability of benzene, or for the fact that the benzene undergoes substitution, rather than addition reactions.

The proposal also doesn't explain the fact that all carbon-carbon bonds are the same length.

Try Problem 5.1 on page 145

EQ: Explain the resonance structure for Benzene.

2. Resonance Structure of Benzene

Benzene is a resonance hybrid of two contributing forms.

Draw the 2 resonance structures of benzene.

All carbon-carbon bonds are the same length, and all bond angles are 120 degrees.

• Bond length of C-C is 154 pm

• Bond length of C=C is 134 pm

• All carbon-carbon bonds in benzene are 139 pm long.

• **EQ.** How do I name and draw the molecular structural and skeletal structure of aromatic compounds?

EQ. How do I name and draw the molecular structural and skeletal structure of aromatic compounds?

Naming aromatic compounds

• 1. Many aromatic compounds have nonsystematic names.

• Refer to table 5.1 on page 147

- Toluene
- Phenol
- Aniline
- Acetophenone
- Benzoic acid
- Benzaldehyde
- o-Xylene
- Styrene

EQ: How do I name and draw the molecular structural and skeletal structure of aromatic compounds?

Naming aromatic compounds

- 2. Monosubstituted benzenes are named in the same way as other hydrocarbons, with benzene as the parent name.
- Bromobenzene C_6H_5-Br ,
- $C_6H_5-CH_2CH_3$,
- Nitrobenzene

EQ: How do I name and draw the molecular structural and skeletal structure of aromatic compounds?

Naming aromatic compounds

Phenyl is used for the $-C_6H_5$ unit when benzene ring is considered as the substituent and benzyl is used for the $C_6H_5CH_2-$ group.

EQ. How do I name and draw the molecular structural and skeletal structure of aromatic compounds?

Naming aromatic compounds

3. **Disubstituted benzenes** are named by the ortho(*o*), meta(*m*), para(*p*) system.

- a. A benzene ring with two substituents in a 1,2 relationship is *o*-disubstituted. Pronounced as 'ortho'
- b. A benzene ring with two substituents in a 1,3 relationship is *m*-disubstituted. Pronounced as 'meta'
- c. A benzene ring with two substituents in a 1,4 relationship is *p*-disubstituted. Pronounced as 'para'

EQ. How do I name and draw the molecular structural and skeletal structure of aromatic compounds?

Naming aromatic compounds

- 4. Benzenes with more than two substituents are named by numbering the position of each substituent.
- a. Number so that the lowest possible combination of numbers is used.
- b. Substituents are listed alphabetically.

EQ. How do I name and draw the molecular structural and skeletal structure of aromatic compounds?

Naming aromatic compounds

- Try These ...
- 5.2 – 5.4 on pages 159

Vocab Review

- Ortho
- Meta
- Para
- Phenyl
- benzyl
- Toluene
- Phenol
- Aniline
- Acetophenone
- Benzoic acid
- Benzaldehyde
- Xylene
- Benzene
- Styrene

EQ: How do I name and draw the molecular structural and skeletal structure of aromatic compounds?

Naming aromatic compounds

- Check HW (5.3 - 5.5 on pages 148-149)
- Try these ...5.22, 5.26 - 5.29 on page 172
- Tomorrow - Naming Aromatic compounds Quiz

Electrophilic Aromatic Substitution of Benzene (EAS)

- EQ: What are the general features of EAS?

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Electrophilic Aromatic Substitution of Benzene (EAS)

- General features of electrophilic aromatic substitution reactions (Section 5.4)
- 1. An electron-poor reagent reacts with the electron-rich aromatic ring.
- 2. Substitution, rather than addition, occurs in aromatic rings.
- 3. A catalyst is needed for substitution reactions.
- 4. The reaction has two steps.
- 5. The product is aromatic.

Electrophilic Aromatic Substitution of Benzene (EAS)

- EQ1. How do I predict the reaction product(s) for the following reactions:
- a) Halogenation (-X)
- b) Nitration (-NO₂)
- c) Sulfonation (-SO₃H)
- d) Alkylation (-R)
- e) Acylation (-COR)
- EQ2. Illustrate and explain the mechanism of the above reactions.

- EQ1. How do I predict the reaction product(s) for a Halogenation reaction?
- EQ2. Illustrate and explain the mechanism of the above reactions.

- Transparency # 37 (fig. 5.5 on page 152)

- EQ1. How do I predict the reaction product(s) for a Halogenation reaction?

Halogenation

Name	Halogenation
Substituent Group	-X (-F, -Cl, -Br, -I)
Reactants: (Benzene + ?)	F ₂ , Cl ₂ , Br ₂ , I ₂
Catalyst	FeX ₃
Product	C ₆ H ₅ -X

- EQ1. How do I predict the reaction product(s) for a Nitration reaction?

Nitration

Name	Nitration
Substituent Group	-NO ₂
Reactants: (Benzene + ?)	HNO ₃
Catalyst	H ₂ SO ₄
Product	C ₆ H ₅ -NO ₂

- EQ1. How do I predict the reaction product(s) for a Sulfonation reaction?

Sulfonation

Name	Sulfonation
Substituent Group	-SO ₃ H
Reactants: (Benzene + ?)	SO ₃ (fuming sulfuric acid)
Catalyst	H ₂ SO ₄
Product	C ₆ H ₅ -SO ₃ H

- EQ1. How do I predict the reaction product(s) for a Alkylation reaction?

Friedel-Craft's Alkylation

Name	Alkylation
Substituent Group	-R
Reactants: (Benzene + ?)	RX
Catalyst	AlX_3
Product	C_6H_5-R

- EQ1. How do I predict the reaction product(s) for a Acylation reaction?

Friedel-Craft's Acylation

Name	Acylation
Substituent Group	-COR
Reactants: (Benzene + ?)	RCOX
Catalyst	AlX_3
Product	C_6H_5-COR

- EQ1. How do I predict the reaction product(s) for a Oxidation reaction?

Oxidation

Name	Oxidation
Reactants: (alkylbenzene + ?)	$KMnO_4$
Catalyst	H_2O
Product	C_6H_5-COOH

- EQ1. How do I predict the reaction product(s) for a Reduction reaction?

Reduction

Name	Reduction
Reactants: (alkylbenzene)	H ₂
Catalyst	Pt, high pressure
Product	alkylcyclohexane

- **Try These...**
- **5.8, 5.9 on page 154**
- **5.10 - 5.11 on page 156**
- **Pages 172-173 - do 5.31, 5.33**

- **Try These...**
- **5.17 on page 162**

- 1. How do substituents affect the reactivity of an aromatic ring?

- 2. How do substituents affect the orientation of the reaction?

Substituent effects in electrophilic aromatic substitution

A. General effects (Refer to Diagram on page 157 and to Fig 5.8 on page 158)

- 1. Substituents affect the reactivity of an aromatic ring.
- 2. Substituents affect the orientation of further substitution.
- 3. Substituents can be arranged in three groups:
 - a. Ortho/para directing activators
 - b. Ortho/para-directing deactivators.
 - c. Meta-directing deactivators.

- Try 5.12, 5.13 on page 158

Substituent effects in electrophilic aromatic substitution

- **B. Explanation of effects**
 1. **Activation and deactivation.**
 - a. All activating groups donate electrons to an aromatic ring.
 - b. All deactivating groups withdraw electrons from a ring.
 - c. Electron donation or withdrawal may be due to inductive or resonance effects.

Substituent effects in electrophilic aromatic substitution

- **B. Explanation of effects (Section 5.8)**
 2. **Orienting effects.**
 - a. **Ortho, para directors.**
 - The intermediates from *o,p* attack are more stable because they can be stabilized by resonance donation by the substituent.
 - b. Any substituent with a positively polarized atom bonded to the ring is a meta director.

- 1. Nitration of Phenol
- 2. Chlorination of Benzaldehyde

- Try 5.14, 5.15 on page 161

Vocab Review

- | | |
|-----------------------|----------------|
| • Kekule's structure | • Toluene |
| • Resonance structure | • Phenol |
| • Aromatic compound | • Aniline |
| • Ortho | • Acetophenone |
| • Meta | • Benzoic acid |
| • Para | • Benzaldehyde |
| • Phenyl | • Xylene |
| • benzyl | • Benzene |

•Organic synthesis

- Organic synthesis (Section 5.11)
- A. To synthesize substituted benzenes, it is important to introduce groups so that they have the proper orienting effects.
- B. It is best to use retrosynthetic analysis to plan a synthesis.

• Polycyclic Aromatic Hydrocarbons

Polycyclic aromatic hydrocarbons consist of two or more fused benzene rings

Naphthalene (2 benzene rings)

Anthracene (3 benzene rings at 180°)

Phenanthrene (3 benzene rings at about 120°)

• Polycyclic Aromatic Hydrocarbons

Naming compounds

• **Polycyclic Aromatic Hydrocarbons**

Naming Anthracene compounds

• **Polycyclic Aromatic Hydrocarbons**

Naming Phenanthrene compounds
