

6.1.1 (a/b/c/d/e/f/g)

colourless, sweet-smelling,
carcinogenic, highly flammable (i)

Benzene Structure

Uses: drugs, dyes, explosives, plastics

Kekulé Model - suggested in 1865



- Ring structure w/ alternating C=C and C-C bonds
- Disproven by:

1. **Resistance to reaction w/ bromine**
 - Doesn't decolourise bromine water in an electrophilic addition reaction under normal conditions

2. **Lower hydrogenation enthalpy**
 - Expected = -160 kJ mol^{-1}
 - Actual = -208 kJ mol^{-1} (more stable)
3. **All bonds same length** - 0.139 nm (discovered 1929)
 - C-C: 0.154 nm
 - C=C: 0.134 nm

unlike C=C alkenes
cyclohex-1,3,5-triene

C₆H₆ - benzene
phenyl - when dominant
Methyl = 1
CH empirical
Mr = 78 and
C₆H₆ molecular
already discovered
attached to - alkyl chain w/ functional group
- alkyl chain of ≥ 7 C atoms

Delocalised Ring Model



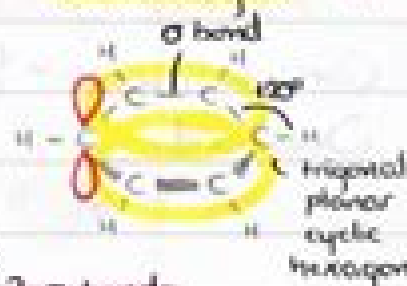
C's other 3 in σ bonds

Stable

- Trigonal planar cyclic hexagon of 6 C's + 6 H's w/ 12 σ bonds
- Sideways overlap of 6 p orbitals (each w/ 1 e⁻) perpendicular to plane of hexagon creates system/ring of delocalised π electron density above and below hexagon
- energetically favourable structure of delocalised π e⁻s in ring system
- reacts w/ electrophiles w/ H substituted
- no addition as not energetically favourable (must disrupt ring structure)

Aromatic Compounds 1

e.g. nitrobenzene
2,4-dichlorobenzene
phenylamine
benzoic acid
benzaldehyde } receptors *



Benzene Reactions by Electrophilic Substitution



uses catalyst + reactant

unstable intermediate

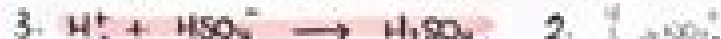
electrophile generated

Mechanisms

always the same

Nitration

uses H⁺ +



overall:



conc. H₂SO₄

30°C

NO₂



+ H₂O

conc. H₂SO₄, 30°C

nitrobenzene limits

- Decolourise bromine water in electrophilic addition reaction
- Due to localised e⁻s in π bond above + below plane of C=C (greater e⁻ density)
- Don't decolourise bromine water in electrophilic addition
- Due to insufficient delocalised π e⁻ density around any 2 C atoms to polarise Br₂ molecule (can w/ halogen carrier)

Arene vs Arene Reactivity

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Dorothy Warren, Neil Dixon



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