- Read Chapter 13.

Prototypical Aromatic Compound: Benzene $C_6H_6$ (isolated from whale blubber)

Structure? 4 degrees of unsaturation (double bonds or rings), but less reactive/more stable than an alkene.

Proposals:

1) Sir James Dewar

\[ \text{Dewar Benzene} \]

Wrong!

2) Albert Ladenberg

\[ \text{Ladenberg benzene} \]

Wrong!

3) Friedrich Kekulé \( \Rightarrow \) Cyclohexatriene

\[ \text{Almost right!} \]

\( \sqrt{1.47 \text{ Å}} \) Alternating single and double bonds

\( \sim 1.33 \text{ Å} \)
Current Understanding of Benzene: (The Right Structure)

1) Regular hexagon
2) All C-C bond lengths = 1.39 Å
3) Each C $\rightarrow$ sp² hybridized

Some double bond character between all C's!

"Quick" Orbital Depiction:

$\left\{ \begin{array}{c}
\text{2p orbitals (all parallel)} \\
\text{Orbital overlap among all neighboring C's.}
\end{array} \right\}$

$\Rightarrow$ DELOCALIZATION of ELECTRONS
$\Rightarrow$ Circle of e- density above & below ring

Delocalization = Stability
How much energy is delocalization worth?

\[ \text{C}_6\text{H}_6 + \text{H}_2 \xrightarrow{\text{Pd}} \text{C}_6\text{H}_{12} \quad \Delta H = -28.6 \text{ kcal/mol} \]

If benzene were 3 isolated alkenes, then

\[ \text{C}_6\text{H}_6 + 3\text{H}_2 \xrightarrow{\text{cat.}} \text{C}_6\text{H}_{12} \quad \Delta H \sim -85 \text{ kcal/mol} \]

In actuality:

\[ \text{C}_6\text{H}_6 + 3\text{H}_2 \xrightarrow{\text{cat.}} \text{C}_6\text{H}_{12} \quad \Delta H = -49.3 \text{ kcal/mol} \]

Energy of stabilization due to delocalization:

\[ 32.9 \text{ kcal/mol} \]

Benzene is \( \sim 30 \text{ kcal/mol} \) more stable than we would expect. AROMATICITY is powerful!