Announcements: 1) Discussion sections, labs & office hours begin this week!
   (Schedule of discussion sections & office hours on course website.)

2) Lab: Canvas website
   Quizzes due by midnight on day before your lab.
   Pre-lab assignment

3) If you are transferring your lab grade from previous semester, please see me after class.

4) Added to course website: notes, practice problems
Recall: Benzene: Extra stability from delocalization of $e^-s$ in the $\pi$-system

How much extra stability? $\sim 30$ kcal/mol

\[
\begin{align*}
\text{H-Br} & \rightarrow \text{HBr}^+ \checkmark \\
\text{H}_2 & \rightarrow \text{H}^+ \checkmark \\
\text{PtO}_2 & \rightarrow \text{Pt}^+ \checkmark
\end{align*}
\]

\[
\begin{align*}
\text{H-Br} & \rightarrow \text{No Rxn!} \\
\text{H}_2 & \rightarrow \text{Very Very Slow} \\
\text{PtO}_2 & \rightarrow \text{No Rxn!}
\end{align*}
\]
Is C₆H₆ the only aromatic compound? **No**.

**4 Criteria for Aromaticity:** Molecule must be:

1) **Cyclic**

2) Fully conjugated → every atom has p orbital parallel to π-system

3) **Planar** (so p orbitals can overlap)

4) **Hückel's Rule:** \((4n + 2)\) π \(e^-\)s, \(n = \text{integer} (0, 1, 2, 3 ...)

**Ex:**  \[\square\]  
1) Cyclic \(\checkmark\)  
2) Fully conjug \(\checkmark\)  
3) Planar \(\checkmark\)  
4) \(\sum \pi_e^- = 4n + 2\) \(\checkmark\)

**Ex:**  \[\square\]  
1) Cyclic \(\checkmark\)  
2) Fully conjug \(\checkmark\)  
3) Planar \(\checkmark\)  
4) \(4 \pi e^- = 4n + 2 \rightarrow n = \frac{1}{2}\) \(\times\)
Why is $4n+2$ so important? Bigger MO picture...

Ethylene

$\pi$-bond = $2pc_1 + 2pc_2$

2 atomic orbitals $\rightarrow$ 2 molecular orbitals

$\pi^*$ 1 node antibonding orbitals

2pc$_1$ - 2pc$_2$

E

$\sigma^*$

2p

C$_1$ 0 nodes bonding orbital

$\Delta E$

2pc$_1 + 2pc_2$
Benzene: 6 2p orbitals → one on each C.

Atomic orbitals → 6 molecular orbitals

3 nodes 2 nodes (antibonding)

Nonbonding level (p-orbital)

1 node → bonding

0 nodes
Frost Magic Circle → Easy → generates MO diagram for π system for aromatic compounds.

Protocol:

1) Draw circle (centered on nonbonding level).
2) Draw ring of molecule w/ vertex/point down.
3) Where ring meets circle → MO (π)
4) Fill in e-s (bottom up)
\[4n + 2 = 4, \ n = \frac{1}{2} \times \text{Anti-aromatic}\]
1) cyclic $\times$

2) fully conjugated $\times$

Substituted benzene $\rightarrow$ only consider aromatic piece

1) cyclic

2) fully conjugated

3) planar

4) $4n+2=6$, $n=1$ $\checkmark$
Polynuclear aromatic = multiple aromatic rings

Naphthalene

1) cyclic ✓
2) fully conj ✓
3) planar ✓
4) $4n + 2 = 10$, $n = 2$ ✓

Aromatic

1) cyclic ✓
2) conj ✓
3) planar ✓
4) $4n + 2 = 10$, $n = 2$ ✓
system

\text{don't count!}

\text{sp}^3

\text{sp}^2

\text{sp}

\text{N}

\text{H}

\text{H}

\text{H}

\text{sp}^3

\text{lp on N to} \text{lp}

\text{4)} \text{f}_{n+2} = 6, \quad n = 1

\text{3) planar}

\text{2) conjugate}

\text{1) cyclic -- "heterocyclic"}
1) cyclic ✓
2) Fully conj ✓
3) planar ✓
4) $\theta = 4n + 2$, $n=1$ ✓

Please note: I forgot to put $\Theta$ on N in lecture. Sorry!