Week 2

Bonding Models

2.1 Bonding Models 1

9/10: • Lecture 1 recap.
  - Aspects of mechanism.
    - Orbitals, energy surface, and kinetics.
    - Masha redraws Figure 1.6.
    - These are the three main pictures that we'll learn about.
  - Today, we'll focus on orbitals.
- Today: Bonding models.
  - Reading: Anslyn and Dougherty (2006), Chapter 1!!
- **Bonding**: How electrons are shared between nuclei.
  - This determines all of molecular structure and reactivity (which is the name of this class, and underpins all of organic chemistry!).
  - From bonding, there arise concepts such as nucleophilicity, electrophilicity, etc.
- There are several levels of bonding theory / models that we'll talk about today.
  - Caveat: *All* of these models are no more than *approximations* of reality that are useful to us.
- Lecture outline.
  1. Lewis structures.
  2. VSEPR.
  3. Valence Bond Theory (VBT).
  4. Molecular Orbital Theory.
  5. Qualitative Molecular Orbital Theory (QMOT).
- Lewis structures.

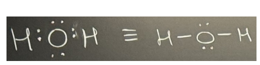


Figure 2.1: Lewis dot structures.

- Developed in 1916 by G. N. Lewis.
  - He was nominated 48 times, but never won the Nobel Prize because some people on the review committee didn't like his "interesting personality."
- In this model, we use dots to — on paper — indicate where electrons are in bonds.
- From these **Lewis dot structures**, people developed the "stick structures" that we still use today.
- Lewis structures are very useful in identifying the number of bonds and lone pairs.

- Valence Shell Electron Pair Repulsion (VSEPR).
  - Developed 1939-1957.
  - Key finding: Electrons in bonds repel each other, so you maximize the distance between bonds.
  - This let us go beyond Lewis structures into things like explaining tetrahedral carbon (and its 109.5° bond angles).
  - Issues develop when we try to rationalize other molecules.
    - For example, isobutane has 110.6° Me−C−Me bond angles. The VSEPR purists will cite "sterics."
    - As another example, NH_3 has 107 H−N−H bond angle. The VSEPR purists will cite "lone pair is big."
  - Really, these were just excuses by the VSEPR purists for a bad model, and what we really needed was a new model.

- Valence Bond Theory (VBT).
  - Developed by Linus Pauling, with his seminal paper in 1931.
    - For this work and some other stuff, he won the Nobel Prize in Chemistry in 1954.
    - To be historically accurate, Pauling built off the work of Heitler and London (1926).
    - However, Pauling was the person to both put everybody else's work all together and be visible enough to take the credit.
    - Additional takeaway from Pauling's biography: Don't make your whole life about your work. For example, Pauling was shunned by many of his colleagues after he got into nuclear proliferation, but now we say he was so brave. He even won the Nobel Peace Prize!
    - Takeaway on Pauling vs. Lewis: It pays to not be a jerk. Lewis died via cyanide poisoning (may have been an accident, but was probably suicide).
  - This is a quantum mechanical (QM) description of Lewis structures.
  - Central tenet: Each atom contributes 1 valence electron in a QM-derived atomic orbital (AO).
    - Shows that electrons are delocalized between atoms, and where two electrons overlap and localize is a chemical bond.
    - In other words, electrons are not restricted to tight orbitals.
  - Many concepts arise within VBT until the advent of MO theory.

- VBT was key for many conceptual innovations, such as **hybridization**, **electronegativity**, and **resonance**.

- **Hybridization**: The mixing of orbitals on the same atom to make new orbitals.
  - Specifically, we can take a linear combination of AO waveforms (or AOs).
  - More directional orbitals give you better overlap and therefore stronger bonds.
  - Example: A linear combination $s + p_y + p_x + p_z$ yields four sp^3-hybridized orbitals. That's four orbitals with uneven lobes. We can draw all of these on top of each other, and from *there*, we get the tetrahedral carbon.

- We always like new models that agree with old models; this is called a **sanity check**.
- We can also calculate something called the **hybridization index**.

- **Hybridization index**: The number i in the following formula, expressed as a function of the experimentally determined bond angle θ. *Denoted by* $\boldsymbol{i}$. *Given by*

$$1 + i\cos\theta = 0$$

  - Example: NH_3 has a hybridization index of 3.4.
  - Example: H_2O has a hybridization index of 4! That's why it has the tiny bond angle. The remaining s-character is localized on the oxygen, and that's why we say that oxygen is electron dense and nucleophilic.
    - Would this similarly predict that H_2O has longer bonds than NH_3??

- **Electronegativity**: The power of an atom to attract electrons to itself.
  - There are different scales for this. We probably used the **Pauling scale**, but there is also a **Mulliken scale**.
  - More electronegative atoms have lower energy orbitals.
    - This is summarized via the **inductive effect**.

- **Inductive effect**: The withdrawing of electron density through σ-bonds.
  - Example: ACN. We think about nitrogen having a partial negative charge and carbon having a partial positive charge. This results in a dipole.
  - Takeaway: Dipoles arise from electronegativity in VBT!

- **Resonance**: The superposition of several Lewis structures.
  - Example: Consider an α,β-unsaturated ketone. Its resonance structure is a zwitterionic intermediate, and a second resonance structure is a different zwitterion. We have three resonance forms, so that predicts more stable than something with less resonance structures. It also identifies our positive and negative reactive sites.
  - Resonance usually happens through π-networks, but it *can* happen through σ-networks.
  - Takeaway: Delocalization of electron density leads to stability.
  - Know your rules for drawing good resonance structures.
    - We only move bonds, not atoms (no nuclear motion).
    - Prefer to have the least separation of charge.
    - Put the more negative charge on the more electronegative atoms.

- Limitations of VBT.
  - Over time, some key experimental findings emerged that VBT coudn't explain. These results motivated people to develop a new model to explain these rare cases.
    - Nowadays, exceptions to VBT are not so rare.
  - Remember: If a model can't explain certain cases, it's not a useful model.
    - Maxim: Not predictive = not useful.

- Here's a list of the limitations of VBT.
  - Doesn't account for unusual stability/instability (e.g., aromaticity and antiaromaticity).
  - No antibonding orbitals (i.e., no explanation of interactions between molecules).
    - When a nucleophile attacks a ketone, the interaction is with the antibonding orbital of the ketone. Forming a new bond involves populating an antibonding orbital.
  - Thursday is all about aromaticity, and modern ways to conceptualize it.

- This leads to the mother of all bonding models, Molecular Orbital Theory.
  - Central tenet: Molecular orbitals (e.g., σ, σ^*, π, π^*) arise from linear combinations of atomic orbitals (in Orgo, this is s & p; we won't consider d-orbital effects so much).
  - We consider the electronic structure of the whole molecule, not just atoms or bonds.
    - We focus on key molecular orbitals such as the HOMO and LUMO.
  - We also get **group orbitals**: Leads into QMOT, which is MOs for prototypical groups.
- MO theory leads to MO diagrams.

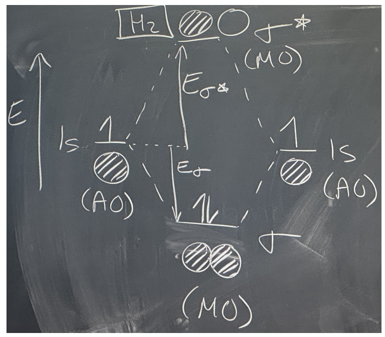


Figure 2.2: MO diagram for H_2.

  - Two atomic orbitals interact to fill two molecular orbitals.
  - We fill the bonding orbital with all the electrons that come in (in this case, 2).
  - The energy of stabilization is E_σ.
  - The destabilization energy is E_{σ^*}.
  - Read Anslyn and Dougherty (2006) for more rules.
  - Notes.
    - $|E_{\sigma^*}| > |E_\sigma|$. Thus, if the antibonding orbitals get populated, the moleucle breaks. This is because of nuclear repulsion.
    - The σ-bond is more stable than the 1s orbitals by themselves. This is why the H$-$H bond forms. This kind of analysis allows us to predict whether or not a bond will form.
  - Question for us to consider: Why doesn't He$-$He form?
    - Because its antibonding MOs would be populated.
- Example MO diagram: Ethylene.

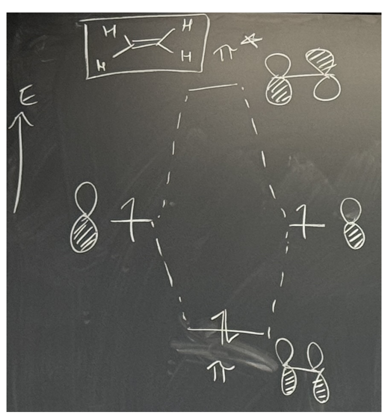


Figure 2.3: MO diagram for ethylene.

- Looking specifically at the π-bond formation.
- This is why we form a stable π-bond.

- Example MO diagram: Formaldehyde.

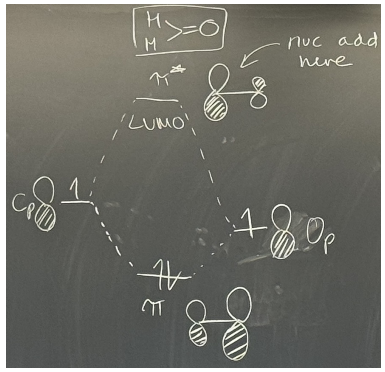


Figure 2.4: MO diagram for formaldehyde.

  - We mix a C_p AO and a (lower energy) O_p AO.
  - These orbitals interact less well than those in ethylene due to their difference in energy.
  - We benefit from constructive phasing, but the lobes are much bigger on oxygen.
  - In the antibonding orbital, the lobes are much bigger on carbon.
  - Principles revealed by this MO diagram.
    - Closer energy AOs give stronger mixing, resulting in lower energy MOs. Lower energy MOs are more stabilizing.
    - More electronegative atoms have lower energy atomic orbitals.
    - The π-orbital is asymmetric because its energetically more similar to O_p than C_p.
      - In other words, it's going to look more like the O_p orbital.
      - One more way of stating this is that the coefficient of oxygen in the LCAO is bigger.
  - We know that the LUMO (frontier orbital) interacts with nucleophiles. The lobe of the LUMO is bigger on carbon, hence why we react there.

- Qualitative MO theory (QMOT).
  - All about forming group orbitals for common functional groups or motifs.
  - Essentially, we may not need to calculate MOs for the whole molecule to find out how every carbonyl reacts; we can trust that carbonyl group orbitals are decently conserved.
  - There are a bunch of rules for how to form a QMOT diagram.
    - See Table 1.7 in Anslyn and Dougherty (2006) for building QMOT diagrams.
  - This is the basis of **Walsh diagrams**.
  - We can build group MOs from linear combinations of s & p AOs.

- **Walsh diagram**: A representation of an MO diagram as a function of geometric distortions.
  - This matters because geometry affects orbital overlap, which can be destabilizing or stabilizing.

- Example QMOT diagram: CH_3.

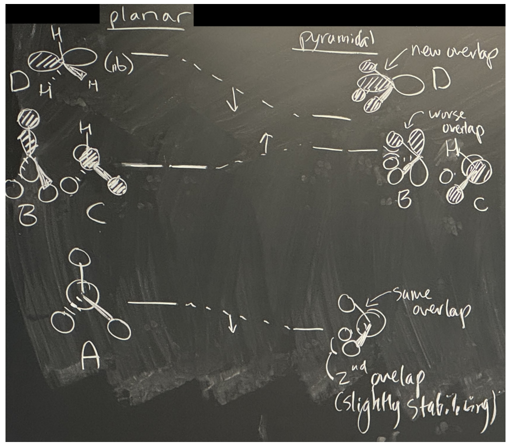


Figure 2.5: QMOT diagram for CH_3.

  - Key question: What geometry of CH_3 is favorable?
  - Masha defines axes.
  - Undetermined yet if this is a radical, cation, or anion. We'll get there!
  - We look at a planar set of orbitals first.
    A. All phases in sync, all s orbitals.
    B. Phases align top to bottom with the p_x orbital of carbon.
    C. Phases align in and out of the board with the p_y orbital of carbon.
    D. Nonbonding; just the p_z orbital.
  - There are also **E**, **F**, and **G** orbitals that are energetically above these, but we won't draw them for now (because we won't fill them with electrons in the carbocation, carbanion, or carbon radical).
    - The **E**, **F**, and **G** orbitals will have the opposite phasing of the lower orbitals!
  - We now draw an analogous, pyramidal set of orbitals.
    A. Overlap is *slightly* more favorable because we have a secondary orbital interaction between the hydrogens now. The C−H overlap stays the same.
    B. Worse overlap. We're losing a **primary** interaction instead of gaining a **secondary** one, so the energy of **B** actually goes up *more* than **A** went down. We also get some destabilizing secondary interaction between the H orbitals.
    C. Just like **B**, we get worse primary overlap, and new interfering secondary overlap.
    D. Gets stabilized the *most* significantly! This is because we've taken something with no bonding interactions and *created* bonding interactions between the p-orbital and the hydrogens.
  - Relationship between QMOT and Walsh diagrams: A Walsh diagram is a QMOT diagram with everything connected.
  - Now how do we fill electrons?
    - Consider the ${CH_3}^+$ cation: We have 6 electrons, so we populate the planar orbitals because it's more stable overall.
    - Consider the ${CH_3}^-$ anion: We have 8 electrons, so we populate the pyramidal orbitals because *they're* more stable overall.
  - This rigorous prediction of conformation is the benefit of this model.
  - We can also use this model for other isostructural molecules.

- Examples.
  - NH_3: 8 electrons, pyramidal.
  - BH_3: 6 electrons, planar.
  - $\cdot CH_3$: 7 electrons, *slightly* planar.
    - ➢ But this is a special case only for $\cdot CH_3$; any other radical is pyramidal.

- **Primary** (orbital interaction): An interaction between orbitals on adjacent atoms in a molecule.
- **Secondary** (orbital interaction): An interaction between orbitals on atoms that are separated by one other atom in a molecule.
- What is quantitative about QMOT?
  - There is a lot more depth in Anslyn and Dougherty (2006). You can calculate the actual potential energy surface and figure out these conformations exactly.
- Example QMOT diagram: CH_2.

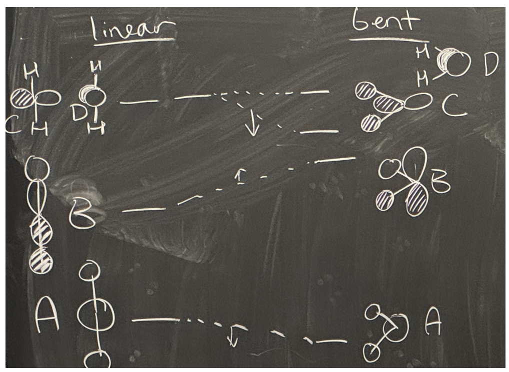


Figure 2.6: QMOT diagram for CH_2.

- Two geometries: Linear and bent.
- Linear.
  A. Linear chain of s-orbitals with matching phases.
  B. Linear chain of matching phases orbitals, with p_x on carbon.
  C. One of the other p-orbitals, with no phasing.
  D. The last remaining p-orbital, again with no phasing.
- Bent.
  A. Goes down slightly. We kept primary, and added secondary.
  B. Losing primary overlap and gaining a destabilizing secondary interaction; higher E like before.
  C. Adding *significant* constructive interference. Biggest effect again!
  D. Staying the same; no bonding interactions to begin or end with. We don't consider secondary interactions when there's no density at all there.
- Example species.
  - H_2O: 8 electrons, bent.
    - ➢ Note that this model predicts that H_2O has nondegenerate lone pairs, which has been experimentally verified!
    - ➢ Bulk water acts as if it has degenerate lone pairs. We can read Anslyn and Dougherty (2006) about this, but otherwise, it's outside the scope of the class.

    - CH_2 (a **carbene**): 6 electrons, a mix of linear and bent!
        - We'll return to carbenes in a few weeks.
        - We'll define **triplet** (2 electrons in different orbitals) and **singlet** (2 electrons in same orbital) carbenes later.
        - Triplet is 136°, and singlet is 105°, so the triplet is more linear and the singlet is more bent! The triplet has reactivity more characteristic of the linear orbital picture, and the singlet has reactivity more characteristic of the bent orbital picture.
        - The triplet is more favored by 9 kcal/mol

- Example QMOT diagram: Formaldehyde.

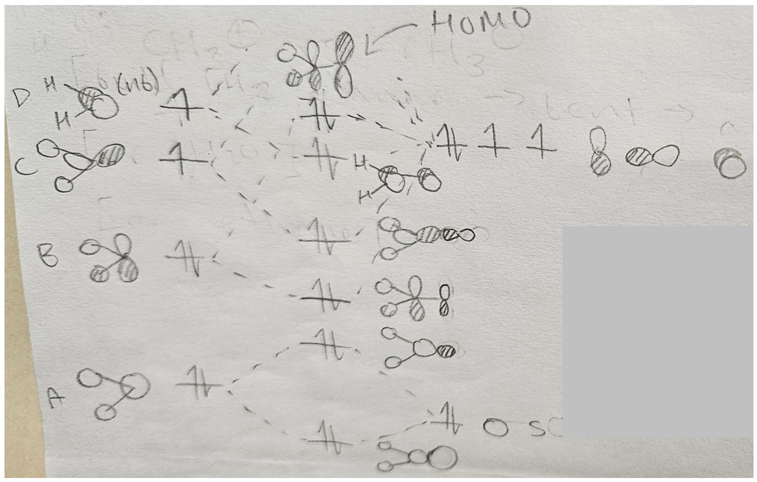


Figure 2.7: QMOT diagram for formaldehyde.

    - The HOMO has a larger coefficient on O; this explains why protonation occurs on O and not C!

- Key takeaway: QMOT diagrams and MO diagrams both make the same predictions about the electronic structure and reactivity of formaldehyde (sanity check).
    - Example: They both predict that carbonyls are nucleophilic on oxygen.
    - Example: Orbital mixing is stronger when orbitals are of similar energy.
    - Example: Orbital coefficients are larger on an atom when the MO is closer in energy to the AO that originates with that atom.
    - Example: Orbitals are lower in energy on more electronegative atoms.
    - Etc.

2.2 Bonding Models 2

9/12:
- Lecture 2 recap.
    - QMOT for formaldehyde (see Figure 2.7).
    - Recall that the HOMO has a larger coefficient on oxygen, which means that protonation occurs on oxygen instead of carbon.
    - No other topics from Lecture 2 are reviewed.
- Today: Bonding models (continued).

- Lecture outline.
  - Huckel theory.
  - Aromaticity.
  - Banana bonds.
  - Wave functions.
- **Huckel theory**: A quick way to build MOs for conjugated π-systems.
  - Qualitatively great and quantitatively bad.
    - Quick and dirty, but generates useful predictions.
    - Not *accurate*, but definitely *useful*.
  - It is used to analyze the connectivity and topology of the π-system in a planar molecule.
  - Key assumptions.
    - The π-system is independent of the σ-network.
    - You only consider valence electrons.
    - Only neighboring orbitals interact, i.e., only π-orbitals on adjacent atoms.
    - We ignore orbital overlap and electron repulsion.
  - These are some wild simplifications, but it is quick and useful!
  - Rules.
    - The number of p-AOs you mix equals the number of new MOs you make.
    - The energy of the new MOs is distributed symmetrically around the **nonbonding energy level**.
    - The number of nodes increases by 1 with each energy level.
    - The MOs reflect the symmetry of the molecule.
- **Nonbonding energy level**: The energy of the nonbonding MOs in a Huckel diagram. *Denoted by* $\boldsymbol{\alpha}$.
  - This is also the energy of an electron in an empty p-AO.
- Example Huckel diagram: Ethylene.

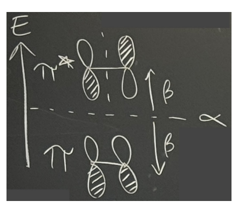
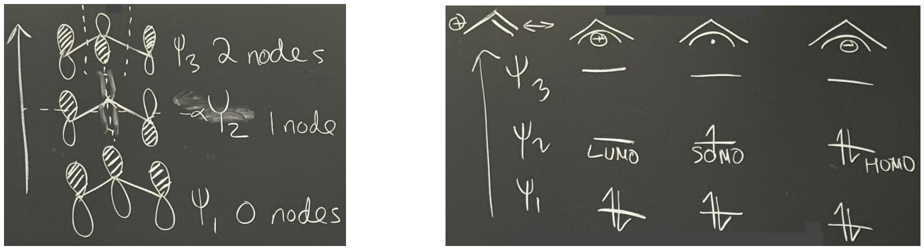


Figure 2.8: Huckel diagram for ethylene.

  - Let's first confirm that this diagram meets all four Huckel theory rules.
    - We get two new π-MOs from two p-AOs.
    - The energy difference from the nonbonding energy level is called β.
    - The number of nodes did increase from 0 to 1.
    - The MOs are symmetric.
  - Thus, this is a valid Huckel diagram!
  - Note: Do remember that symmetric splitting is *not* accurate!
    - On Tuesday, we (correctly) learned that destabilization energy > stabilization energy.

- Example Huckel diagram: Allyl groups.



(a) Diagram. (b) Filling orbitals.

Figure 2.9: Huckel diagram for allyl groups.

  - The lowest energy orbital is called ψ_1.
    - It has 0 nodes.
  - The middle energy orbital is called ψ_2.
    - To maintain symmetry, we have to delete the middle orbital and give opposite phases.
  - The highest energy orbital is called ψ_3.
    - It has the 2 nodes we expect.
  - We now fill electrons for the allyl cation, radical, and anion (Figure 2.9b).
    - These species have 2, 3, and 4 electrons, respectively.
  - Now let's look at where each of these species will react.
    - Nucleophiles will attack the LUMO of the cation.
    - Radicals react with their SOMO (singly occupied molecular orbital).
    - Electrophiles will engage the HOMO of the allyl anion.
  - But the LUMO, SOMO, HOMO are all ψ_2!
    - ψ_2 has no density at the middle carbon, so all of these species should only react at the terminal carbons.
    - This prediction of Huckel theory is experimentally confirmed!
    - Intuitively, reacting at the terminals allows you to keep the double bond in play; thermodynamically, you wouldn't want to cleave it by reacting in the middle.

- Example Huckel diagram: Benzene.

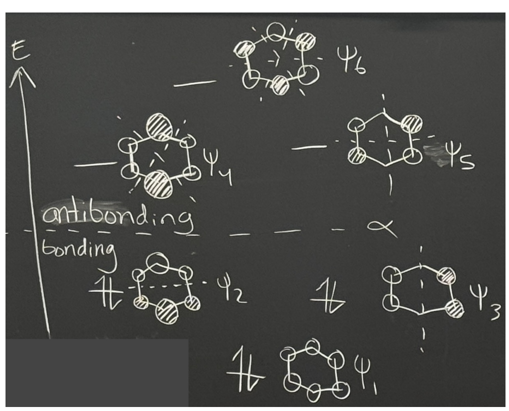


Figure 2.10: Huckel diagram for benzene.

- For cyclic systems, we draw a **Frost circle**.
  - For benzene, the radius of the Frost circle is 2β.
- We create $\psi_1, \dots, \psi_6$.
  - ψ_2, ψ_3 and ψ_4, ψ_5 are degenerate.
  - No electron density on the central p-orbitals in ψ_3 implies bigger coefficients on the corresponding orbitals in ψ_2.
    - ➢ See Anslyn and Dougherty (2006) for more!!
  - ψ_4, ψ_5 have 2 nodes at angles.
  - For ψ_6, we have 3 nodes through a hexagon, which is alternating shading.
- α is the nonbonding level; higher is antibonding, lower is bonding.
- 6 electrons in benzene's bonding π-system yields stabilization.
  - In particular, we observe stabilization relative to three ethylenes: An extra 36 kcal/mol of stabilization!
  - Huckel theory can't really compare energy between two molecules; β is more a qualitative parameter than a quantitative one.

- **Frost circle**: A circle in which we inscribe a regular n-gon with one point down — where n is equal to the number of carbons in the cyclic system — that is used as a guide for drawing Huckel orbitals.
- Example Huckel diagram: Cyclobutadiene.

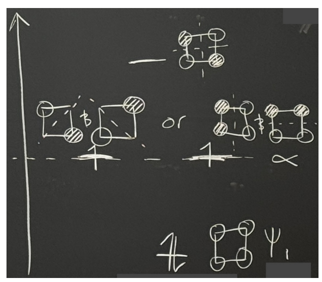


Figure 2.11: Huckel diagram for cyclobutadiene.

- ψ_1 has no phase inversion and no nodes.
- There are two different ways to draw the orbitals for ψ_2, ψ_3.
  - We can dive deeper into this difference in Anslyn and Dougherty (2006).
- No extra stability relative to three ethylenes!
- The model also predicts a ground-state triplet diradical.
  - Indeed, this molecule is highly reactive and dimerizes spontaneously at 35 K.

- We now do a deep dive into aromaticity.
- The history of aromaticity.
  - In 1855, Hofmann (not Hoffmann) coins the term "aromatic" because these compounds were smelly.
  - In 1861, we have Kekulé's dream of a snake eating its tail.[1] This inspired a circle of electrons.
  - In 1925, Robinson describes aromaticity as extra stabilization of a molecule.
  - In 1931, Huckel puts forth **Huckel's rule**.

[1] "At least, Kekulé *said* it was a dream!" - Masha. Good use of reasonable doubt and objectivity in her thinking!

- **Huckel's rule**: Cyclic, planar molecules with $4n + 2$ continuous π-electrons are aromatic.
  - If you have $4n$ electrons in a cyclic planar molecule with continuous π-electrons, then you are antiaromatic (extra unstable).
  - Thus, these molecules usually distort out of the plane to break antiaromaticity and become nonaromatic.
    - Both cyclobutadiene and cyclooctatetraene are antiaromatic. Cyclooctatetraene bends into a boat so that its π-orbitals are pointing toward each other.
  - No phase inversions are allowed; we must connect orbitals without crossing the σ-plane.
    - What does this mean??
- Features of aromatic compounds.
  - Aromatic stabilization energy (36 kcal/mol).
  - Equalization of the bond lengths.
    - Essentially, the bond lengths do not alternate but rather share an identical bond order of 1.5.
  - Ring currents and magnetic properties.
    - Those interested in polymer chemistry might be interested in exploiting these properties!
    - Specifically, these are properties that come from a sea of electron density.
  - Benzene vs. hexa-1,3,5-triene.
    - In benzene, all bond lengths are 1.40 Å.
    - In hexa-1,3,5-triene, the single bonds are 1.45 Å, the terminal double bonds are 1.34 Å, and the internal double bond is 1.37 Å.
    - The bond lengths of benzene equalize because benzene has two equally stable major resonance structures.
      - This is why we often draw benzene as a hexagon with a circle in the middle: This is actually the most accurate picture of it!
    - The bond lengths of hexa-1,3,5-triene do *not* equalize because the only resonance structure we can draw of it is a zwitterion, and thus will be a minor contributor.
  - Different kinds of reactivity.
    - Example: Electrophilic aromatic substitution.
    - This is very much distinct from alkene addition chemistry.
- **Möbius aromaticity**: Aromatic rings have one phase inversion (PI), like in a Möbius strip.

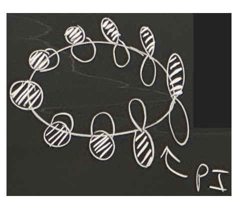


Figure 2.12: Möbius aromaticity.

  - This is a different definition of aromaticity.
    - We could research aromaticity for the rest of our lives if we wanted to.
    - There's a whole field of research devoted to it, and we should look into it if we're interested!!
    - A good starting point is Ajami et al. (2003).
  - The single phase inversion is called a **Möbius topology**.

  - Your PI happens at the sole node.
    - This one node is allowed in Möbius aromaticity, but not in Huckel aromaticity
  - The Möbius topology predicts that compounds are aromatic if they have $4n$ electrons and antiaromatic if they have $4n+2$ electrons.
  - To be clear, this content is outside the scope of this class, but Masha wants us to know about it and be able to research it if we so choose.
- Ring current.

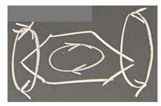


Figure 2.13: Ring current.

  - Suppose you have an external magnetic field perpendicular to the σ-plane.
    - This would induce the π-electrons to rotate through their MOs.
    - These rotating electrons would then create an additional magnetic field.
    - This new magnetic field would *reinforce* the external magnetic field outside the aromatic ring and *oppose* the external magnetic field inside the ring.
    - The strength of the induced magnetic field is proportional to the current (i.e., the size of the ring).
  - Application (NMR): Ring protons are deshielded (higher δ) outside and shielded (lower δ) inside.
    - Cyclohexene: No ring current, so we get a bit of downfield shift for the vinyl protons (δ 5.6).
    - Benzene: Has a ring current, so we get a noticeable downfield shift (δ 7.3).
    - [18]annulene: Has a large ring with many π-electrons, so we get a significant downfield shift for the external protons (δ 9.3) and a significant *upfield* shift for the internal protons (δ −2.9).
- **Quadrupole**: Two dipoles aligned such that there is no net dipole.
  - Example: The dipole aligned up and down in benzene, as opposed to (for instance) the linear dipole in fluoromethane.
  - Lots of applications beyond the scope of this class, but we can look into it if we want.
- **Banana bond**: A bent chemical bond that contains an unusually high concentration of p-character.
  - The bent p-lobes of banana bonds look like bananas (see Figure 2.14), hence the name.
- Example banana bonds: Cyclopropane.

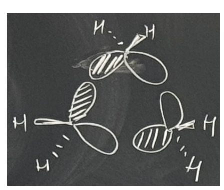


Figure 2.14: Banana bonds in cyclopropane.

  - Cyclopropane needs more p-character because of its 60° bond angles; p-character helps bonds bend.
    - Specifically, the C−C bonding orbitals in cyclopropane are sp^5-hybridized.

- The excess of p-character in the C−C bonds means that the C−H bonds of cyclopropane have correspondingly more s-character.
  - This makes the C−H bonds in cyclopropane shorter than usual!
  - Indeed, there is something of a "conservation" of bonding character: The s-character that's not in the σ-bonds has to go somewhere.
- Group orbitals (HOMO) degenerate.
  - The **Walsh orbitals** have more π-character, so cyclopropane is sp^2-like.
  - This means it is a good π-donor and a bad π-acceptor.
  - Example of donation: The isopropylcyclopropane cation is very stable because all of the sp^2-character is getting donated into the carbocation's empty orbital.
  - What is going on here??

- Wave functions.
  - Review Anslyn and Dougherty (2006), Chapters 4 & 14!!
    - Also look up your Gen Chem or Quantum notes if it's been a while.
  - All bonding theories draw upon QM descriptions of electrons as waves existing in **orbitals**.
- **Orbital**: A wave function that is a specific solution to the **Schrödinger equation**.
  - Masha draws the $1s, 2s, 3s$ orbital penetration graph, as well as what these orbitals look like.
  - Recall that orbitals have **lobes** and **nodes**!
- **Schrödinger equation**: The following equation, where E is the energy of the electron, ψ is the wave function describing the position of the electron in space, and H is the **Hamiltonian operator**. *Given by*

$$H\Psi = E\Psi$$

  - ψ^2 is the probability of finding an electron in a specific position (i.e., the electron density!).
  - Big Ψ is the total molecular wave function, and little ψ is a molecular orbital.
- **Hamiltonian operator**: A representation of all forces acting on the system, such as the kinetic energy of the electron and nucleus, nuclear-nuclear repulsion, electron-electron repulsion, etc.
- Next week, we'll talk about DFT and approximating solutions to the Schrödinger equation. It will be like an intro to computational chemistry!
- Example: Electron density in H_2 MOs.
  - Masha redraws Figure 2.2 to start, and Figure 7.3 from Labalme (2023).
  - The point is that...
    - The bonding MO has a lot of electron density between the nuclei, even though you still have some at the atoms;
    - The antibonding MO has minimal to no electron density between the nuclei; the AOs (ϕ_1^2, ϕ_2^2) are very separate.