

# CHE 1301

## Basic Principles of Modern Chemistry I

### Week 9

Hi! Thanks for checking out the weekly resources for Chemistry 1301! This resource covers topics typically taught by professors during the 9<sup>th</sup> week of classes.

Visit our website, <https://baylor.edu/tutoring>, to sign up for appointments and check out additional resources for your course! You'll find helpful links with the following titles:

- "Online Study Guide Resources" – The pace of your course may vary slightly from what's shown in this document. If you don't see the topics you're learning right now, use this link to find the weekly resources for the rest of the semester.
- "How to Participate in Group Tutoring" - See if there is a Chemistry 1301 group tutoring session being hosted this semester. These are weekly question/answer sessions taught by our master tutors!
- "View tutoring times for your course" or "Schedule a private 30-minute appointment!"

You can also give us a call at (254)710-4135, or drop in! Our hours are Monday-Thursday 9 am – 8 pm on class days.

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**KEY WORDS: Polarity, Sigma & Pi Bonds, Molecular Orbital Theory, Percent Yield**

### TOPIC OF THE WEEK: Polarity

*How do I tell whether a molecule is polar?* (Notes here on determining overall direction of dipole too!)

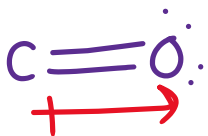
A molecule is polar if, overall, one side of the molecule is more charged than the others. This is significant because a polar molecule can be attracted to other polar molecules, or to ions. Keep in mind: even if there are some dipoles (think: some atoms are hogging the electrons), a molecule might not be polar! Here are some steps you can follow to determine polarity:



- 1) Draw the Lewis structure. Determine the electron geometry and make sure your drawing is adjusted to match this! Step 3 will show why this is so important.
- 2) Look for dipoles! Follow steps a-b for each bond:
  - a. Figure out which of the two atoms is more electronegative. This atom is better at keeping electrons close to it, so the shared electrons (from the bond) will spend more time with this atom than the other.



- b. Draw an arrow next to the bond that points toward the more electronegative atom. Make the head of the arrow look like a plus sign



- 3) See if the dipoles cancel. In other words, look for symmetry. Then, determine polarity as follows:

Conditions	Polar	Nonpolar Option 1	Nonpolar Option 2
Dipoles present	Yes	No	Yes
Symmetric	No	Either way	Yes

- a. How do I know if the dipoles cancel? If they are exactly opposite each other, they will cancel.

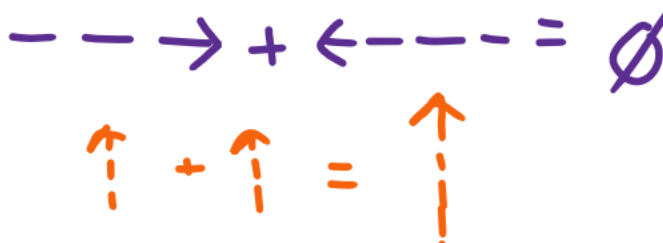


- b. **TO DETERMINE DIRECTION OF OVERALL DIPOLE:** Add them all up as you would vectors:

- i. Sketch the **components**. The “horizontal component” is a horizontal line that goes from the **head** of the vector to the *x-coordinate* of the **tail** (arrow end). The vertical component is a vertical line that goes from the **head** of the vector to the *y-coordinate* of the **tail**. I’ll use another example here, since carbon dioxide’s dipoles cancelled out.

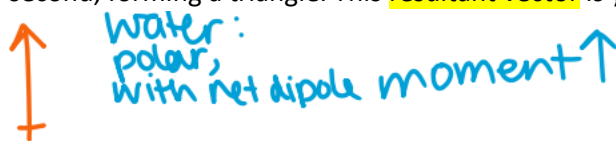


- ii. Add the **horizontal components** to each other. This vector will be the horizontal component of the **overall dipole**. Add the **vertical components** to each other. This vector will be the vertical component of the **overall dipole**.



- iii. If neither component is zero, draw the horizontal component of the overall dipole. Then, start at the tail end of the horizontal component, and draw the vertical component. Connect the head of the first arrow to the tail of the

second, forming a triangle. This resultant vector is your overall dipole.

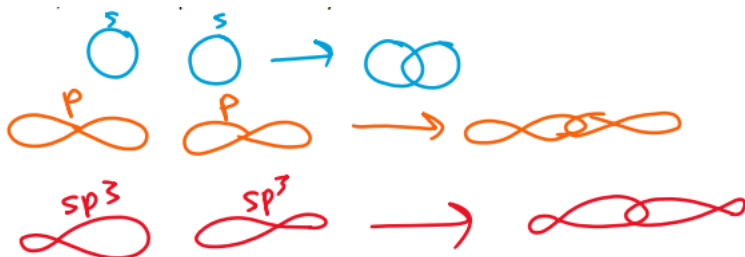


## Highlight 1: Sigma and Pi Bonds

Review: quantum numbers.

A **sigma bond** is “head-on” overlap, and a **pi bond** is “side-by-side” overlap. The difference between the two is that a sigma bond occurs along the line connecting the two nuclei, and a pi bond does not—there is a node along the line connecting the two nuclei.

A **single bond** is a sigma bond. This is the only thing strong enough, by itself, to keep two atoms together. A sigma bond can be the overlap between 2 s orbitals, the overlap between 2 p orbitals, or the overlap between two hybrid orbitals.

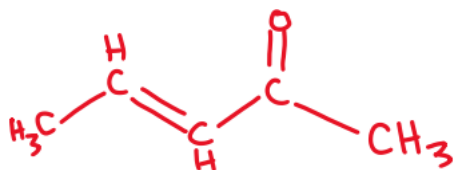


A **double bond** includes a sigma bond, and it also has a pi bond. There are two different pairs of orbitals that are overlapping, which makes the connection between the atoms stronger! Since more electrons are “keeping them together,” the two atoms involved in a double bond will be closer than the two involved in a single bond. Similarly, the atoms in a triple bond will be even closer to the two involved in a double bond.

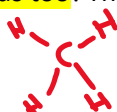
A pi bond is the sharing of electrons between p orbitals when the two are parallel to each other.



A lot of the questions that you’ll be asked on this subject are similar to this example: How many sigma and pi bonds are contained in the following structure?



Make sure you **count the condensed hydrogen bonds too!** They form single bonds to whatever atom they are written next to. So,  $\text{H}_3\text{C}-$  means



1. **Calculate the number of sigma bonds:** (# of single bonds) + (# of double bonds)
  - a. Include the condensed C-H bonds!
2. **Calculate the number of pi bonds:** (# of double bonds) + 2(# of triple bonds)


Where do these formulas come from? Each single bond has one sigma bond (only). Each double bond has one sigma bond and one pi bond. Each triple bond has one sigma bond and 2 pi bonds.

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## Highlight 2: Molecular Orbital Theory

Molecular orbital theory describes the positioning of electrons when bonds are formed. It is built on the **atomic orbital theory** and **hybridization theory**—it tells us what the **combination** of these atoms' orbitals will look like when they overlap with each other (which is when a bond is formed).

When orbitals overlap, either **sigma** or **pi** bonds can form. However, orbitals can either overlap constructively or destructively. You've heard it said that an electron has characteristics of a wave. Well, because of this, we can describe orbitals as having phases. This means that the graphs describing their behavior can be shifted to the right or left. Note: The graphs don't actually look like the ones shown below. However, the concepts of constructive and destructive interference are the same! And these concepts are the only things necessary to memorize.

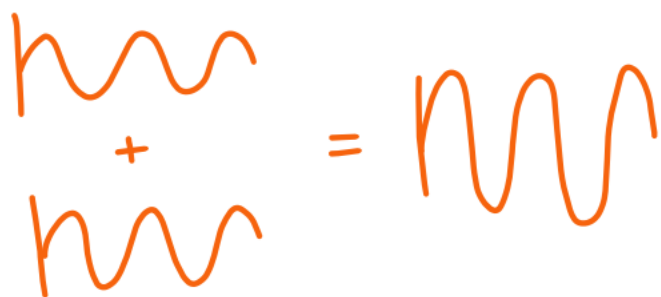


a possible "description" for an orbital

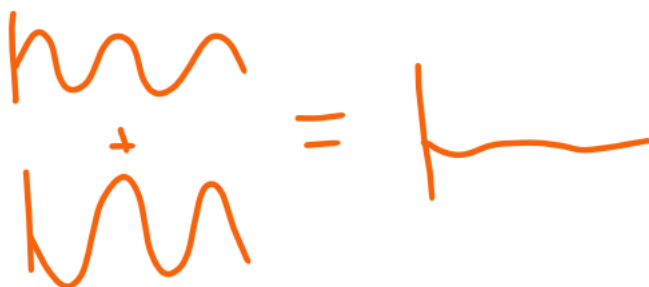


a "description" for another possible orbital

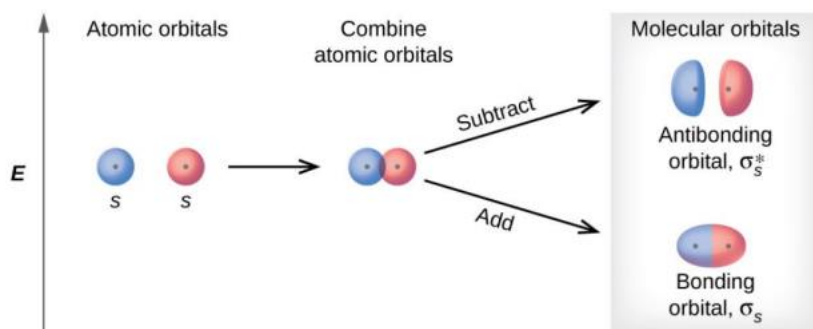
If, when the two orbitals overlap, their functions have the **same phase**, they will **interfere constructively** with each other. Their functions will add to each other, creating a larger orbital. This is called a **bonding orbital**.



If, when they overlap, their functions have **opposite phases**, they will **interfere destructively** with each other. Their functions will take away from each other. The resulting orbital is called an **antibonding orbital**.

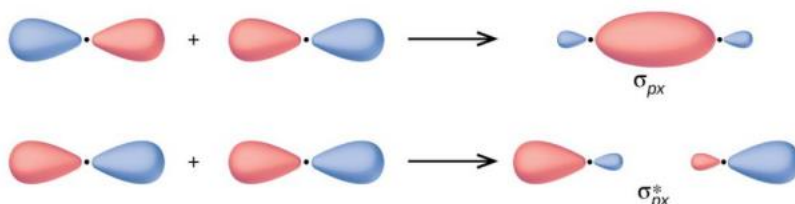


So, let's look at the various possible outcomes from the combination of orbitals. We'll start with the **overlap of two s orbitals**. They'll overlap head-on, forming a sigma bond (see Highlight 1). If they are in the same phase when they do this, they'll form a bonding orbital, as shown below. If they're in opposite phases, they'll form an antibonding orbital.

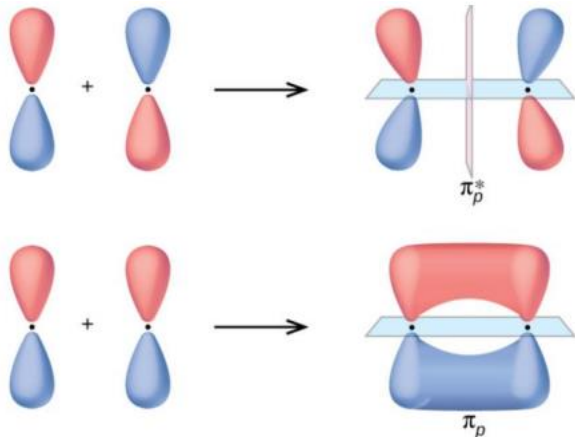


I took this figure (and the rest of the ones in this doc) from this website, which has an excellent explanation of MO theory: [Molecular Orbital Theory – Chemistry \(hawaii.edu\)](http://www.hawaii.edu/chem/mo) Check it out for a more thorough explanation!

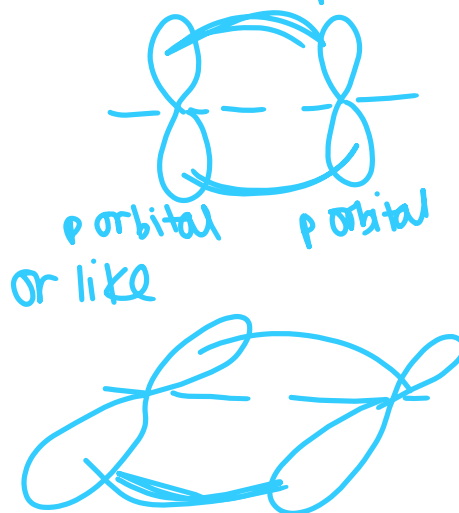
Now, let's look at p orbitals. They can overlap in two ways (see Highlight 1 to review pi bond formation). If they overlap in a head-on fashion, they can either form **sigma bonding orbitals** (lobes of the same phase are overlapping) or **sigma antibonding orbitals** (lobes of the opposite phase are interacting), just like the s orbitals.



If they are parallel when they overlap, they can either form pi bonding orbitals or pi antibonding orbitals. There are *two possible directions in which this could occur* (two different ways the p orbitals could be perpendicular to the sigma bond), so there will be **2 bonding pi orbitals and 2 antibonding!**

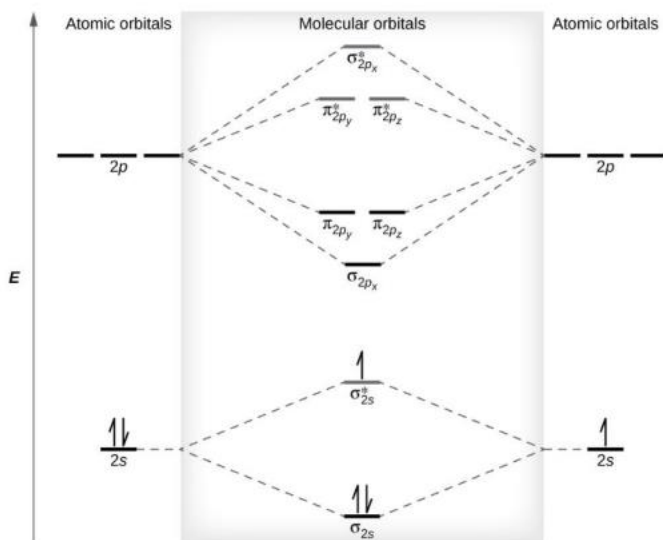


can overlap like



Drawing a molecular orbital energy diagram:

1. Draw the energy diagrams for each atom—see Week 6 to review this process! Put one atom's energy diagram at the **very left** of your diagram, and put the other at the **far right**. You **only need to include the valence levels**, because these are the ones that will be involved in bonding.
2. **In the middle, draw the possible combinations of each orbital.** S orbitals can form bonding or antibonding sigma orbitals, p orbitals can form bonding or antibonding sigma orbitals OR bonding or antibonding pi orbitals, etc.
  - a. The vertical positioning of these orbitals is shown below. The *orbitals that take the least energy to sustain are furthest down*. **Bonding orbitals will always take less energy** than the original orbitals (think: electrons like to be paired!) **But antibonding orbitals take more energy** to sustain than the original orbitals. Since the phases repel each other, it's like trying to push two magnets together with the wrong sides facing each other.



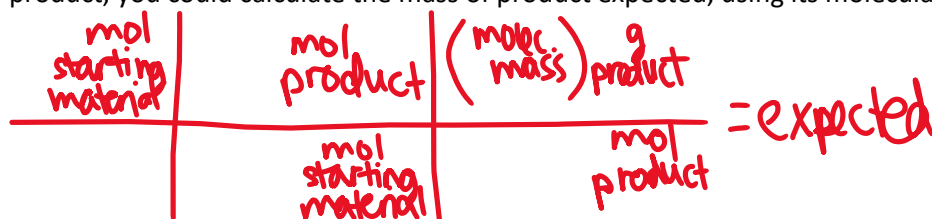
3. Fill in electrons bottom to top, least energy to most! Check and make sure that the number of orbitals you started with equals the number of orbitals you finished with.

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## Highlight 3: Percent Yield

Here's a formula you should know! It's not super related to the other topics we covered, but it is very related to stoichiometry, which we talked about last week.

The percent yield compares the amount of material collected from an experiment is from the amount that you expected to collect, based on stoichiometric calculations. For example, if you knew you had put one mole of starting material into a reaction, and that each mole of starting material made two moles of product, you could calculate the mass of product expected, using its molecular mass:



Then, you could calculate % yield = observed/expected \* 100.

Here are some steps:

1. Calculate expected values—review stoichiometry from Week 3.
2. Use that formula!

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## Check Your Understanding

1. Is NH<sub>3</sub> polar? Hint: Make sure you've accounted for VSEPR theory in your Lewis diagram!
2. Draw the MO diagram for O<sub>2</sub>.
3. You expected 100 g of product. After your experiment, you weighed the product and discovered that you had made 83 g. What is your percent yield?

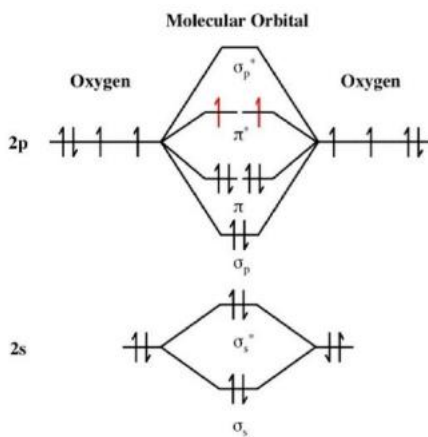
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## Things You May Struggle With

- Keep in mind: having dipoles does not mean that a molecule is polar. Polarity means that, overall (after adding dipoles), one side of the molecule is more charged than the other. So, if a molecule has dipoles, but they cancel each other out, it will not be polar. Try the Check Your Learning questions to make sure everything's making sense!
- Single bond vs. sigma bond, double bond vs. pi bond: A single bond is classified as a sigma bond. A double bond contains two bonds; one of them is a sigma, and one is a pi.

That's all this week! Please reach out if you have any questions and don't forget to visit the Tutoring Center website for further information at [www.baylor.edu/tutoring](http://www.baylor.edu/tutoring). Answers to Check Your Learning are below.

1. Yes, NH<sub>3</sub> is polar!



- 2.
3. 83%

[O2 Molecular Orbital Diagrams | 101 Diagrams](#)