

CHE 1301

Basic Principles of Modern Chemistry I

Week 7

Hi! Thanks for checking out the weekly resources for Chemistry 1301! This resource covers topics typically taught by professors during the 7th 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.

KEY WORDS: VSEPR, Valence Bond Theory, Hybridization

TOPIC OF THE WEEK: Molecular Bonding Theory

How is this all connected? It can be really tricky to keep track of which theory applies to which idea, because what we accept as true today is a combination of several theories! As each theory is introduced, look out for a sentence or two explaining its niche.

A main part of bonding theory is studying the 3D geometry of electrons in a molecule. One of the theories necessary for these predictions is called VSEPR.

Highlight 1: Valence Shell Electron Pair Repulsion (VSEPR) Theory

Main Idea: Electron groups (lone pairs or bonds) will "try" to get as far away from each other as possible, since electrons are negative, and like charges repel.

Calculating VSEPR:

1. Count the number of lone pair electron groups.

- Count the number of **bonding electron groups** (single bonds, double bonds, and triple bonds all count as one group).
- Determine molecular geometry using the table on page 2!

How the table below was created: This goes back to the main idea summarized above. Say that there are 2 electron groups around an atom. What's **the greatest angle that these two groups could have between them?** Well, it would be if they're in a straight line, or 180 degrees from each other. This geometry is called **linear**. *You'll notice that the table does not have an option for 1 bonding pair and one lone pair. Why is this? Because it wouldn't satisfy the octet/duet rule!*

The same is true when considering an atom with three electron groups around it. To find the greatest possible number of degrees that can be allowed between groups, divide the number of degrees in a circle (360 degrees) by 3. There will be 120 degrees between each group. Actually, this rule can be generalized:














Bond angle for molecule with **2 or 3 groups of bonding electrons:**

$360/n$, where n = number of electron groups

The molecule with 3 groups of bonding electrons is called **trigonal planar**.

So what happens if one of the groups is a lone pair? Greater electron density results in greater repulsion, and **lone pairs** have greater electron density (think: their groups will need more space) than single bonds. The same is true for **double and triple bonds**. Whenever one of these groups is present (especially lone pairs!), **the other bond angles will have to decrease to give them more room.**

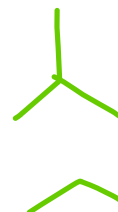
TABLE 5.5 Electron and Molecular Geometries

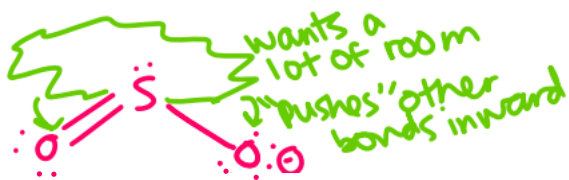
Electron Groups*	Bonding Groups	Lone Pairs	Electron Geometry	Molecular Geometry	Approximate Bond Angles	Example
2	2	0	Linear	Linear	180°	$\text{:}\ddot{\text{O}}=\text{C}=\ddot{\text{O}}\text{:}$ 
3	3	0	Trigonal planar	Trigonal planar	120°	$\begin{array}{c} \text{:F:} \\ \text{:F}-\text{B}-\text{F:} \\ \text{:F:} \end{array}$ 
3	2	1	Trigonal planar	Bent	<120°	$\text{:}\ddot{\text{O}}=\text{S}-\ddot{\text{O}}\text{:}$ 
4	4	0	Tetrahedral	Tetrahedral	109.5°	$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{H} \\ \\ \text{H} \end{array}$ 
4	3	1	Tetrahedral	Trigonal pyramidal	<109.5°	$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{N}-\text{H} \\ \\ \text{H} \end{array}$ 
4	2	2	Tetrahedral	Bent	<109.5°	$\text{H}-\ddot{\text{O}}-\text{H}$ 
5	5	0	Trigonal bipyramidal	Trigonal bipyramidal	120° (equatorial) 90° (axial)	$\begin{array}{c} \text{:Cl:} \\ \\ \text{:Cl}-\text{P}-\text{Cl:} \\ \\ \text{:Cl:} \end{array}$ 
5	4	1	Trigonal bipyramidal	Seesaw	<120° (equatorial) <90° (axial)	$\begin{array}{c} \text{:F:} \\ \\ \text{:F}-\text{S}-\text{F:} \\ \\ \text{:F:} \end{array}$ 
5	3	2	Trigonal bipyramidal	T-shaped	<90°	$\begin{array}{c} \text{:F:} \\ \\ \text{:F}-\text{Br}-\text{F:} \\ \\ \text{:F:} \end{array}$ 
5	2	3	Trigonal bipyramidal	Linear	180°	$\text{:F}-\text{Xe}-\text{F:}$ 
6	6	0	Octahedral	Octahedral	90°	$\begin{array}{c} \text{:F:} \\ \\ \text{:F}-\text{S}-\text{F:} \\ \\ \text{:F:} \end{array}$ 
6	5	1	Octahedral	Square pyramidal	<90°	$\begin{array}{c} \text{:F:} \\ \\ \text{:F}-\text{Br}-\text{F:} \\ \\ \text{:F:} \end{array}$ 
6	4	2	Octahedral	Square planar	90°	$\text{:F}-\text{Xe}-\text{F:}$ 

*Count only electron groups around the central atom. Each of the following is considered one electron group: a lone pair, a single bond, a double bond, a triple bond, or a single electron.

Let's apply that idea that greater electron density results in greater repulsion. What would happen if there were 3 electron groups around an atom, but one of them was a lone pair?

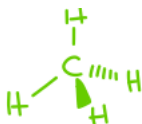
1. Calculate what angles would be if all groups were single bonds
2. The **electron geometry** will be the same overall shape. (The lone pair is an electron group, just like the bonds, and it will occupy one of the three spaces). **Molecular geometry** looks at the geometry of the bonds only and ignores the lone pair.
3. The angles immediately next to the "high-density" group will be greater than they were. The others will be less.



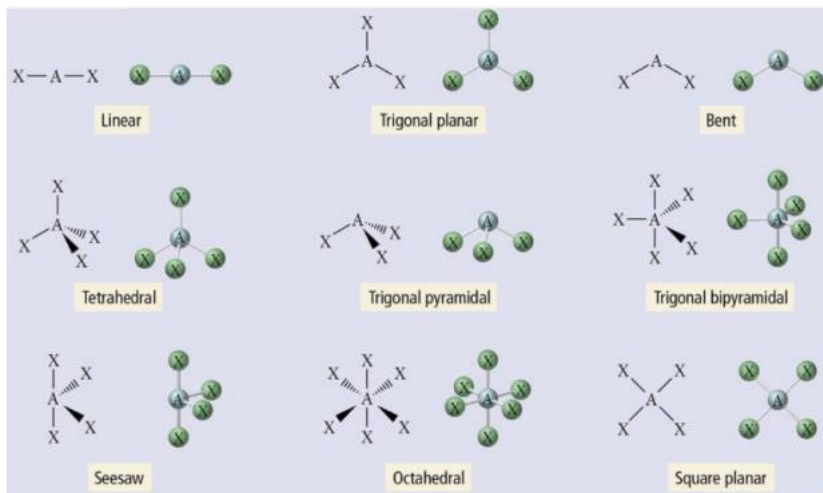


Why doesn't that double bond "push" back and make up for the strong lone pair? Well, it does push back more than the single bond, but it's not enough. Lone pairs are very assertive about having their own space!

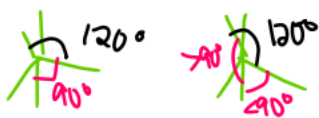
Now we reach the row that has four electron groups. You might think that there would be 90 degrees between, but the atom can do even better than that, because it can use 3D space! In other words, it can move one of its electron groups out of the plane of the paper... and the other can be pushed into the plane of the paper.



(Side note: Wedge = comes out of the plane of the paper. Dash = goes into the plane of the paper. See this diagram:



Now, try applying these same concepts to the rest of the table! One more time—the electrons will want to be (1) as far apart as possible, and (2) even farther as electron density increases. Look at the molecule with trigonal bipyramidal molecular geometry. What would happen if you tried to increase the angle between the axial and equatorial positions? Other angles would end up decreasing:



Here's a video showing some model kits that make things easier to visualize!

<https://www.youtube.com/watch?v=nxebQZUVvTg>

Highlight 2: Valence Bond Theory

How is this all connected? Molecular geometry is something that we can look at (via x-ray crystallography, for example); VSEPR is a theory to explain it. But VSEPR doesn't cover the way that the bond itself is formed. Where exactly are the electrons when they are "shared" between atoms?

We've discussed electron configuration, or the locations of electrons around an atom. (Check out Weeks 4 & 6 to review this topic). How does this atomic orbital theory lead into molecular orbital theory? In other words, how do atomic orbitals become bonds?

Valence bond theory says that the **overlap of valence electrons' orbitals** leads to the formation of bonds. A covalent bond is the sharing of electrons; when one electron's space overlaps with another's, the overlapped space represents the electrons' belonging to each of the two atoms.

An excellent video lesson on valence bond theory: <https://www.youtube.com/watch?v=Vqx9a2aU99c>

Here's an example: CH₄

1. Draw **valence orbitals** according to **electron configuration**



2. Valence orbitals containing one electron can **interact with each other to pair up their electrons**



But do you notice something weird? According to this picture, **it looks like carbon should only be able to form 2 bonds, because it has 2 half-filled valence shells... but it forms 4** (review binding capacity).

And didn't we learn that an atom with four electron groups is tetrahedral? This picture of carbon doesn't look tetrahedral; its p orbitals are only 90 degrees apart.

It turns out that there is an intermediate step missing from valence bond theory. It's explained by what's called hybridization.

Highlight 3: Hybridization

So let's discuss hybridization, which (remember to think about how this is all connected) combines molecular geometry (VSEPR) with the valence bond theory.

Hybridization theory states that, to have the most opportunities to bond at the lowest cost of energy, atoms combine some or all of their valence orbitals to form new, degenerate, half-filled orbitals.

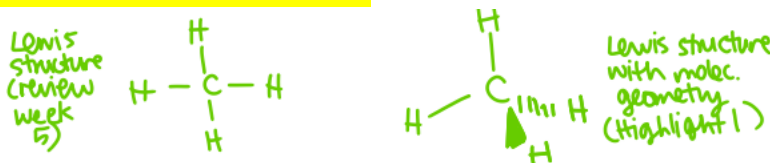
Stepwise (with CH₄ as an example),

1. Atoms exist separately, all their electrons at ground states



2. Some or all of the valence orbitals combine, or hybridize.

- a. How do you know how many? This depends on how many electron groups you see. The **number of electron groups = number of orbitals hybridized**. We'll talk about double/triple bonds in a moment. Importantly, the **number of orbitals hybridized = number of new orbitals formed**.

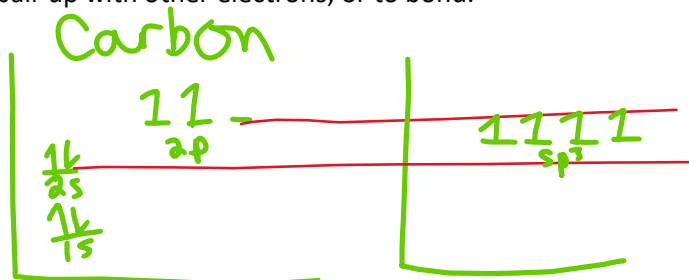


- b. So what are the new orbitals like? They will have some of the characteristics of each of the orbitals that they are made of. If an s orbital combines with 2 p orbitals (to give 3 sp² hybrids), the new orbitals will have 33% s character and 66% p character. They'll be kind of round, like an s orbital, but mostly p-shaped.

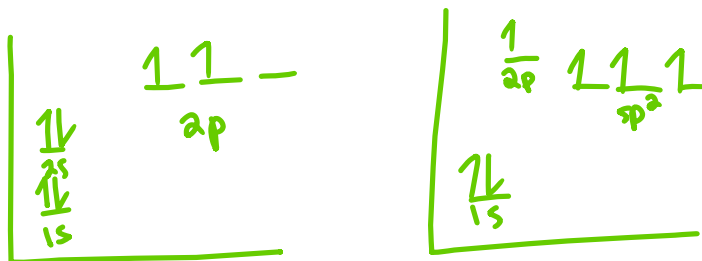


- c. How does this solve the problem? The new orbitals will arrange themselves as far away from each other as possible. (Unhybridized s and p orbitals' locations are not as far from each other as possible.) This satisfies VSEPR theory! And one other important note explains the atom's increased bonding capability...

3. Now that the orbitals' energies are close together, atoms' electrons can be promoted and/or demoted such that each of them is in its own orbital. Now, all these electrons have the ability to pair up with other electrons, or to bond.



4. So what if some orbitals get hybridized but not all? Say that there are 3 electron groups in a structure, but there were 4 valence electron orbitals to start. One of the higher energy orbitals will be left behind.



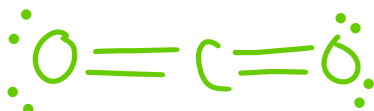
P-orbitals (like the one leftover in the right-hand diagram) are responsible for the formation of pi bonds. Sigma bonds are “head-on,” but pi bonds form between orbitals alongside each other.

Check out this video for a more in-depth explanation of sigma and pi bonds! [Hybridization of Atomic Orbitals - Sigma & Pi Bonds - Sp Sp2 Sp3 - YouTube](#)

And here’s an excellent summary of the sp^3 hybridization discussed above: [sp³ hybridization | AP Chemistry | Khan Academy - YouTube](#)

Check Your Understanding

In this molecule,



1. What is the hybridization of C?
2. What is the molecular geometry of C? O?
3. What is the electron geometry of C? O?

Things You May Struggle With

- *Don’t mistake the tetrahedral bond angle for 90 degrees! Since 3D space can be utilized, it is actually 109.5—see Highlight 1!*
- *A common misconception: Does a larger molecule (one with more than one central atom) have an electron geometry? It doesn’t have one electron geometry—the molecule doesn’t have an electron geometry—but each of its atoms does!*
- *Check out “How is this all connected?” at the beginning of each highlight to make sure you know the differences between the theories.*

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. Answers to Check Your Learning are below.

1. sp (2 electron groups = 2 orbitals hybridized, 2s and 2p. The other 2 p-orbitals will remain unhybridized and will result in double bond formation)
2. Linear, N/A (only one group)
3. Linear, trigonal planar (3 groups)