

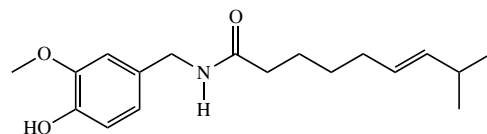
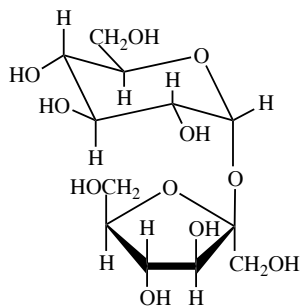
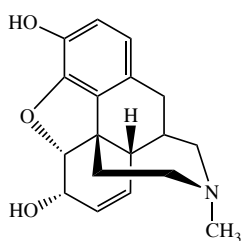
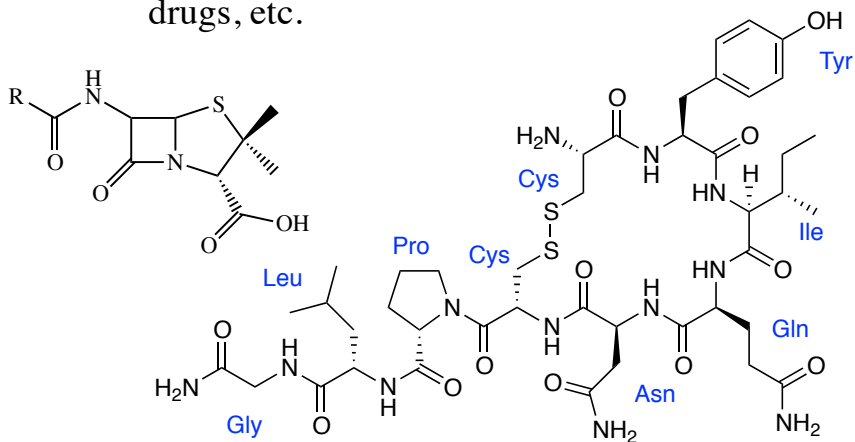
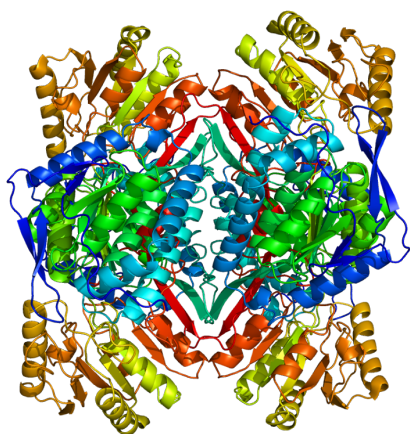
# Lecture Notes Chem 51A

## S. King

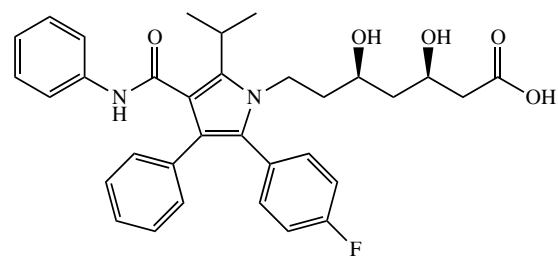
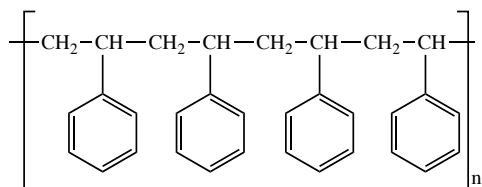
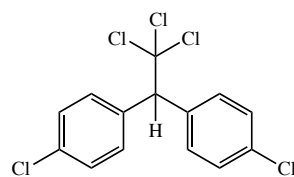
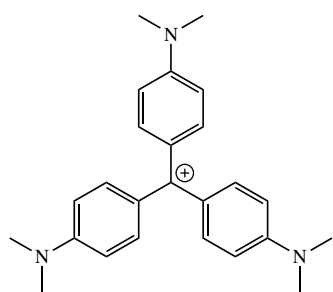
### Chapter 1 Structure and Bonding

Organic Chemistry: **The chemistry of compounds that contain carbon**  
>95% of all chemical compounds are organic.

Naturally occurring organic molecules: hormones, enzymes, carbohydrates, proteins, drugs, etc.



Synthetic organic molecules: rubber, dyes, pesticides, rayon & nylon, drugs, etc.



## **\*\*STRUCTURE DETERMINES REACTIVITY\*\***

### **I. The Structure of an Atom**

All matter is composed of the same building blocks called atoms. An atom consists of a *very dense* nucleus surrounded by electrons that spread through out a relatively *large* volume of space. The nucleus contains protons & neutrons.

**Mass proton:**

**Mass neutron:**

**Mass electron:**

**FUN FACT**

If the nucleus was the size of a ping pong ball:

- It would have a mass of 2.5 billion tons
- The electrons would be on average a mile away

Atomic number: gives # protons in the nucleus

Mass number: sum of the protons and neutrons

*Look @* Carbon:

**Q.** Why does carbon have an uneven mass number?

**A.** In nature elements are usually found as mixtures of isotopes. Three isotopes of elemental carbon are carbon-12 ( $^{12}\text{C}$ ), carbon-13 ( $^{13}\text{C}$ ) and carbon-14 ( $^{14}\text{C}$ ).

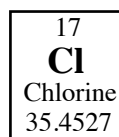
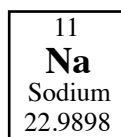
Isotopes have the same number of protons, but different numbers of neutrons:

How is  $^{14}\text{C}$  used to date artifacts?

The half-life of  $^{14}\text{C}$  is 5730 years. Carbon dioxide containing  $^{14}\text{C}$  is continuously made in the atmosphere. A living plant consumes this carbon dioxide during photosynthesis and incorporates the carbon, including  $^{14}\text{C}$ , into its molecules. As long as the plant lives, the  $^{14}\text{C}$  content in its molecules remains the same as in the atmosphere because of the plant's continuous uptake of carbon. As soon as the tree is cut down to make a wooden tool, or a cotton plant is harvested to make fabric, it stops taking in carbon. There is no longer a source of  $^{14}\text{C}$  to replace that lost to radioactive decay, so the material's  $^{14}\text{C}$  content begins to decrease. So, if a wooden tool found in an archeological dig shows a  $^{14}\text{C}$  content of half that found in currently living trees, then it is 5730 years old!

Atoms can also be charged:

- A *cation* is positively charged and has fewer electrons than its neutral form.
- An *anion* is negatively charged and has more electrons than its neutral form.



## II. Bonding

Bonding is the joining of two atoms. Through bonding, atoms achieve a complete outer shell of valence electrons.

**The Octet Rule:** Atoms transfer or share electrons in such a way to attain a filled shell of electrons (the electron configuration of a noble gas such as He, Ne, or Ar).

H:

2nd row elements:

There are *two ways* that atoms can interact to attain noble gas configurations:

## IONIC BONDING & COVALENT BONDING

### A. Ionic Bonding

Atoms attain a filled valence shell by transferring electrons from one to another.

Ionic bonding is seen with atoms of **WIDELY** differing electronegativities:

I							VIII
<b>H</b> 2.2	II						<b>He</b>
<b>Li</b> 1.0	<b>Be</b> 1.6	III	IV	V	VI	VII	<b>Ne</b>
<b>Na</b> 0.9	<b>Mg</b> 1.2	<b>B</b> 1.8	<b>C</b> 2.5	<b>N</b> 3.0	<b>O</b> 3.4	<b>F</b> 4.0	<b>Ar</b>
<b>K</b> 0.8	<b>Ca</b> 1.0	<b>Al</b> 1.5	<b>Si</b> 1.9	<b>P</b> 2.2	<b>S</b> 2.6	<b>Cl</b> 3.2	<b>Kr</b>
						<b>Br</b> 3.0	<b>Xe</b>
						<b>I</b> 2.7	

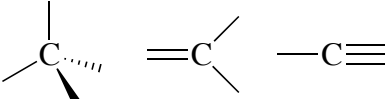
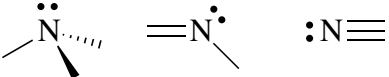
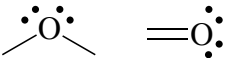

- ❖ IN GENERAL: If electronegativity difference is greater than *about* 1.8, the electron will be transferred completely (the bond will be ionic.)

## B. Covalent Bonding

Atoms attain a filled valence shell by sharing electrons.

★ *This type of bonding is seen with atoms of the same or closer electronegativities.*

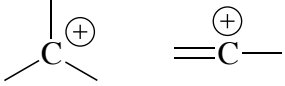
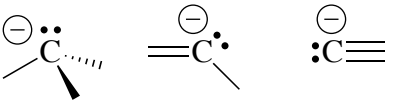
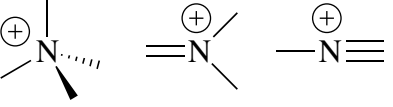
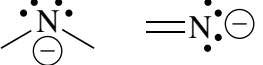
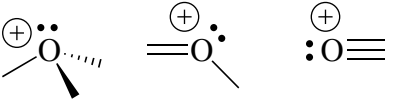
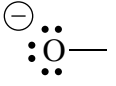
*Look* at how C, H, N, O, & the halogens satisfy the octet rule:

Atom	Valence Electrons	To Complete Shell	Number of Bonds in <i>Neutral</i> Compounds
Carbon (C)	4	4 e <sup>-</sup> needed	4 
Nitrogen (N)	5	3 e <sup>-</sup> needed	3 
Oxygen (O)	6	2 e <sup>-</sup> needed	2 
Hydrogen (H)	1	1 e <sup>-</sup> needed	1 H—
Halogens	7	1 e <sup>-</sup> needed	1 

EZ way to remember: **HONC-1234 rule:**

**H**ydrogens and **H**alogens make 1 bond  
**O**xxygen makes 2 bonds  
**N**itrogen makes 3 bonds  
**C**arbon makes 4 bonds

When C, H, N, O, & the halogens deviate from the HONC rule, they are said to have a **formal charge**. A **formal charge** is a charge associated with an atom that does not exhibit the expected number of valence electrons.

Atom	# Bonds to neutral atom	# Bonds to Atom when Cationic	# Bonds to Atom when Anionic
Carbon (C)	4	3 	3 
Nitrogen (N)	3	4 	2 
Oxygen (O)	2	3 	1 

*How do we know this?*

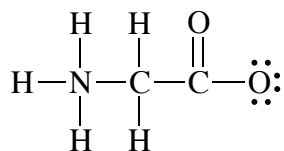
**Formal charge can be determined in three ways:**

1. Memorize the chart above.
2. Calculate by using a formula.

**Formal charge** = (# valence e-s) - (1/2 # bonding e-s) - (# nonbonding e-s)

3. Compare the expected number of valence electrons to the actual number of electrons in the structure.

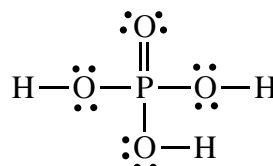
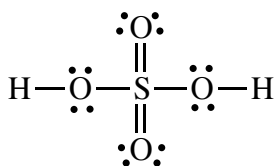
Example: Assign formal charge to any atoms that are charged in the following molecule.



Exceptions to the octet rule:

1. **Third row and higher elements** - These have *d* orbitals available for bonding, so they *sometimes* exceed an octet in their valence shell.

**Examples:** Sulfuric Acid ( $\text{H}_2\text{SO}_4$ )     *and*     Phosphoric acid ( $\text{H}_3\text{PO}_4$ )



2. **Molecules with open shells** - sometimes there are not enough electrons to provide an octet!

**open shell compounds:** can accept a pair of electrons to complete an octet

### III. Representation of Structure

There are different ways to represent the structures of molecules, and some ways provide more information than others:

#### A. Molecular formula $[\text{C}_2\text{H}_5\text{O}]^+$

Molecular formula is useful for calculating molar mass, but it gives no information about how atoms are bonded together. It also doesn't give any information about the location of any formal charges in the molecule.

#### B. Condensed structure

This is the condensed structure of the same compound:



Condensed structures are a shorthand way of drawing molecules where some or all of the covalent bonds are left out. They are drawn in a way that gives information about how the atoms are bonded together.

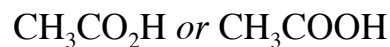
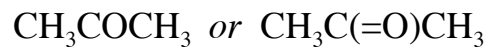
Guidelines:

- All atoms are drawn in, but bond lines are generally omitted.
- Atoms are usually drawn next to the atoms to which they are bonded.
- Parentheses are used around similar groups bonded to the same atom.
- Lone pairs are usually omitted.
- Formal charges are shown on the atom to which they belong.

Examples:







### C. Lewis Structure

Lewis structures give connectivity and the location of all bonding and non-bonding electrons as well as formal charges. They do *not* give information about the three-dimensional (3-D) orientation in space.

*Lewis structure of sample compound:*

Lone pairs are **required** in Lewis Structures! In most other structures they are left out and “understood”, which means that they are *implied*: you understand that they are there, you are just leaving them out to save time.

### D. 3-D Structures

3-D give the three-dimensional orientation in space and all formal charges.  
Lone pairs are optional.

- = in the plane of the paper
- ◄ = out of the plane of the paper
- ⋯ = behind the plane of the paper

## E. Skeletal (Bond-Line) Structures

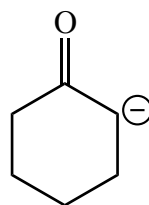
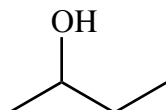
Skeletal structures are a simplified way of drawing more complex molecules, especially those containing rings.

Guidelines:

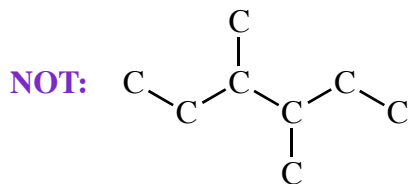
1. Assume there is a carbon at the junction of any 2 lines or at the end of any line.
2. Assume there are enough hydrogens around each carbon to make it tetravalent.
3. Draw in all **heteroatoms** (atoms other than C) and the hydrogens directly bonded to them.
4. Carbon atoms in a straight chain are drawn in as a zig-zag.
5. Lone pairs are often left out and are “understood.”
6. **Always** include formal charges!

*Skeletal structure of sample compound:*

Example: Redraw the following compounds showing all atoms, lone pairs and formal charges



- *Notice: Lone pairs are not required in skeletal structures!* They are implied. You must be able to fill them in where necessary.
- **Keep in mind:** When drawing a molecule, either show all of the hydrogens and all of the carbons or draw skeletal structure. You cannot draw the carbons without drawing the hydrogens!



- It is common to combine more than one type of structure:

## IV. Drawing Lewis Structures

Traditional method:

1. Arrange atoms in the proper orientation (condensed structures will give information about how atoms are bonded together).
2. Sum valence electrons for all atoms. For charged molecules: Add one electron for each *negative* charge, and subtract one electron for each *positive* charge.
3. Distribute electrons by placing bonds between atoms (one bond is two electrons). Use remaining electrons to satisfy the duet rule for H and the octet rule for second row elements. Third row elements can exceed an octet.
4. If all valence electrons are used and an atom does not have an octet, form multiple bonds where possible.

- Maximize the number of bonds without exceeding the octet rule.
- Assign formal charge to any charged atoms.
- Be sure to draw all lone pairs!

Alternative method: Use the HONC-1234 rule for neutral compounds.

\*\*Recommendation: If you have a charged compound, always count electrons!

**Example 1:** Write the Lewis Structure for  $\text{CH}_3\text{Cl}$ .

1. Traditional method:

2. **Shortcut:** Follow the HONC-1234 rule for neutral molecules. For charged structures, use the table given.

**Example 2:** Write the Lewis structure for ethylene ( $\text{CH}_2\text{CH}_2$ ).

**Example 3:** Write the Lewis Structure for  $\text{CH}_3\text{CHOH}^+$

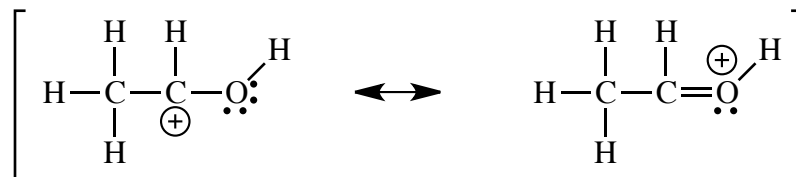
Curvy arrows: show movement of a pair of electrons.

Tail: begins at the current position of electrons

Head: new position of electrons

### Important points about this example:

1. The above molecule can be represented by more than one Lewis structure. The two Lewis structures are *resonance structures* for the same molecule.



- \* Resonance Structures differ only in the arrangement of electrons, **NOT** in the connectivity.
- \* The actual structure of the molecule is a *resonance hybrid* of the 2 structures.

### Arrow Review:

resonance arrow

equilibrium arrow

reaction arrow

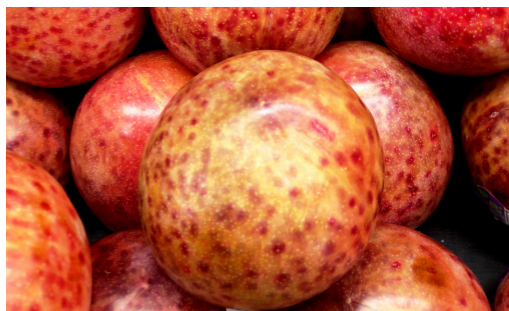
curvy arrow - shows movement of a pair of electrons

fishhook arrow - shows movement of a single electron

Analogy:



+



One way we can approximate the true structure of this molecule is to draw a hybrid structure.

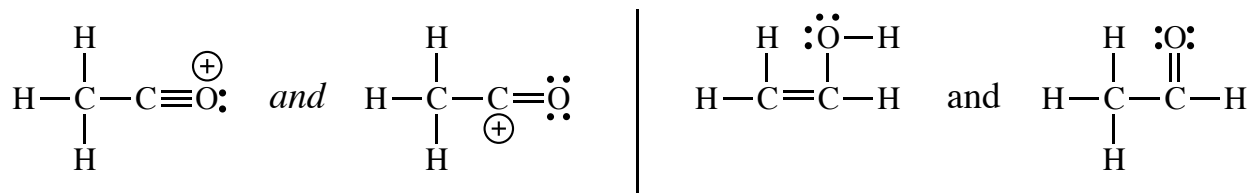
To draw a hybrid structure:

1. Draw all of the single bonds in the molecule.
2. Draw dotted lines for  $\pi$  bonds that are changing location or not showing in every resonance structure.
3. Draw partial charges for charges that are changing location or not showing in every resonance structure using the symbol delta:  $\delta+$  and  $\delta-$
4. To make this easier, you can leave out lone pairs.

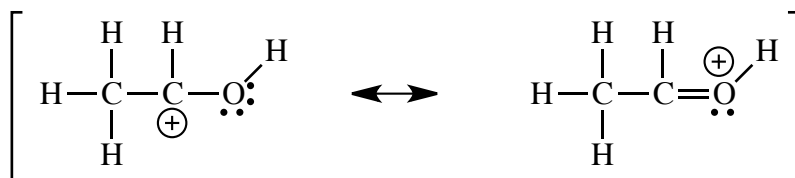
\*\* This hybrid structure gives a more accurate representation of the true distribution of electrons in the molecule. Notice in the hybrid there are two atoms that share the positive charge, that is, there are two sites in the molecule that are electron deficient.

### Important points about resonance structures:

- Resonance structures are *not* real. An individual resonance structure does not accurately represent the structure of the molecule or ion. Only the hybrid does.
- Resonance structures are *not* in equilibrium with each other. There is no movement of electrons from one form to another.
- Resonance structures are *not* isomers. Two isomers differ in the arrangement of *both* atoms and electrons, whereas resonance structures differ *only in the arrangement of electrons*.



2. These two resonance structures are not equivalent:



Q. What makes a good resonance structure?

A. The best resonance structures are the most stable!

Look for the following structural features (*in order of importance*):

Rule #1: Resonance structures w/ more bonds and fewer charges are more stable.

Rule #2: Resonance structures in which every atom has an octet are more stable.

Rule #3: Resonance structures that place a negative charge on a more electronegative atom are more stable.

Additional points:

- ❖ It is okay to have carbon with less than an octet in a resonance structure, but *never* draw O, N or the halogens without an octet.
- ❖ Don't draw resonance structures with a 2+ or 2- charge! These are extremely minor and should not be included.
- ❖ NEVER, EVER exceed an octet for second row elements.

#### IV. Determining Molecular Shape (Geometry)

A Lewis structures tells us which atoms are connected to each other, but it implies nothing about the geometry. *Valence Shell Electron Repulsion (VSEPR)* can be used to predict the geometry of a molecule.

## VSEPR theory:

- The number of groups surrounding a particular atom determines its geometry.  
*A group is either an atom or a lone pair of electrons.*
- The most stable arrangement keeps these groups as far away from each other as possible.

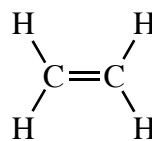
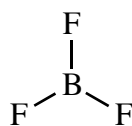
Molecules with **four groups** will adopt a *tetrahedral* arrangement  
Molecules with **three groups** will adopt a *trigonal planar* arrangement  
Molecules with **two groups** will adopt a *linear* arrangement

*Here's a general chemistry example and an organic chemistry example of each:*

### Molecules with two groups:



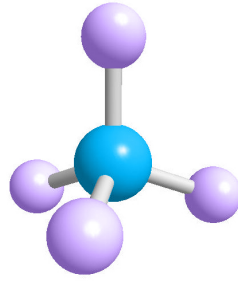
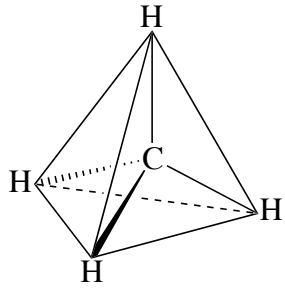
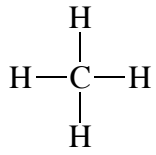
### Molecules with three groups:



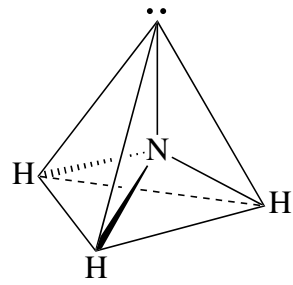
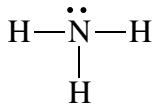
### Molecules with 4 groups:



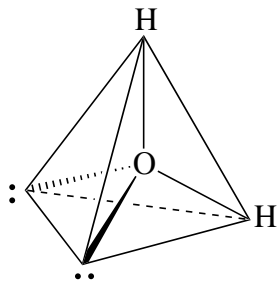
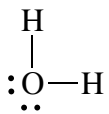
methane:



ammonia:



water:



### Important points:

- Molecular shape (geometry) describes the orientation of the atoms in a molecule. *Lone pairs are not included when naming geometry.*
- Lone pairs (non-bonding electrons) take up more space than the electrons in a bond. This condenses the bond angles from the ideal  $109.5^\circ$ .

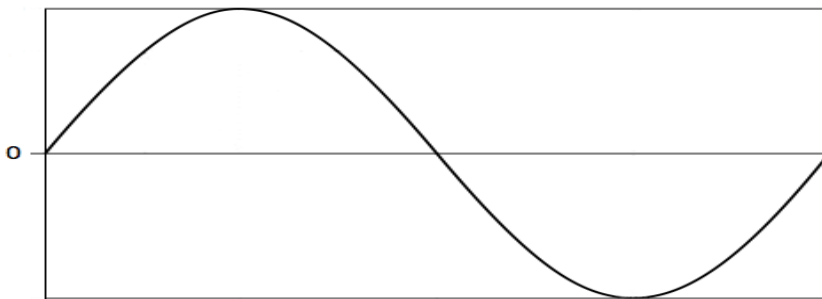
## V. Describing the Orbitals Used in Bonding

In order to understand structure completely, we have to not only be able to describe the geometry of a molecule, but we also need to know the orbitals used for bonding. First we will look at the distribution of electrons, and then we will look at how the atoms combine to form a new covalent bond.

### A. Distribution of Electrons in an Atom

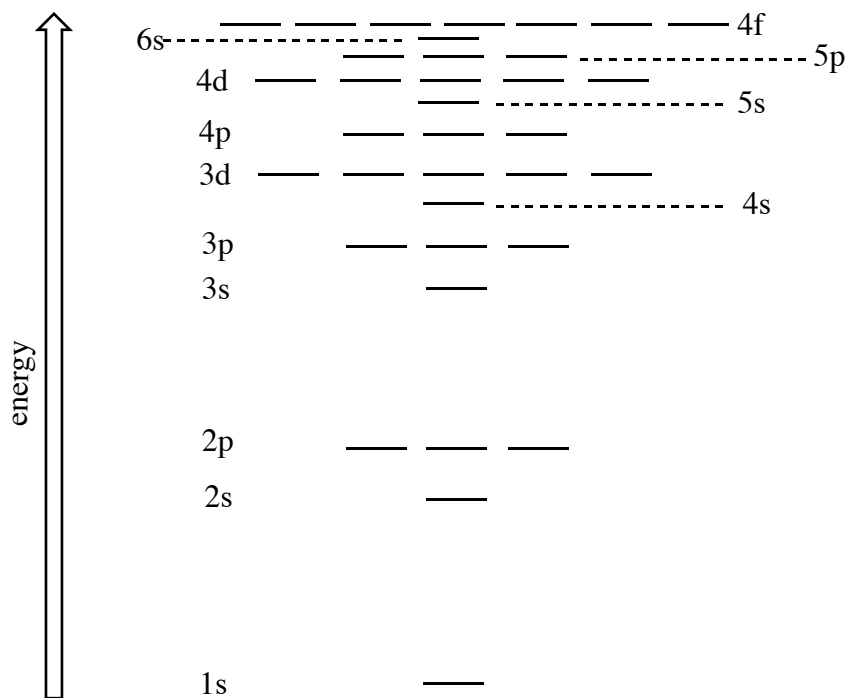
Electrons have wavelike and particle-like properties. Quantum mechanics describes the wavelike characteristics of an atom:

- The exact position of an electron cannot be specified; only the probability that it occupies a certain region of space can be specified (**Heisenberg Uncertainty Principle**)
- A wave function ( $\Psi$ ) is used to describe the motion of an electron in an atom or molecule.



- (+) and (-) **Do not** imply charge. These are the phase of the wave function.
- The square of the wave function ( $\Psi^2$ ) gives the probability of finding the electron at a given distance and direction from the nucleus. Plots of  $\Psi^2$  in three dimensions generate the shapes of s, p, d & f atomic orbitals.
- The electrons in an atom can be thought of as occupying a set of concentric shells that surround the nucleus. Each shell contains subshells, which are the atomic orbitals.

- The energy of the atomic orbitals can be plotted:



***Important points:***

- Each orbital can hold two electrons.

1<sup>st</sup> shell:

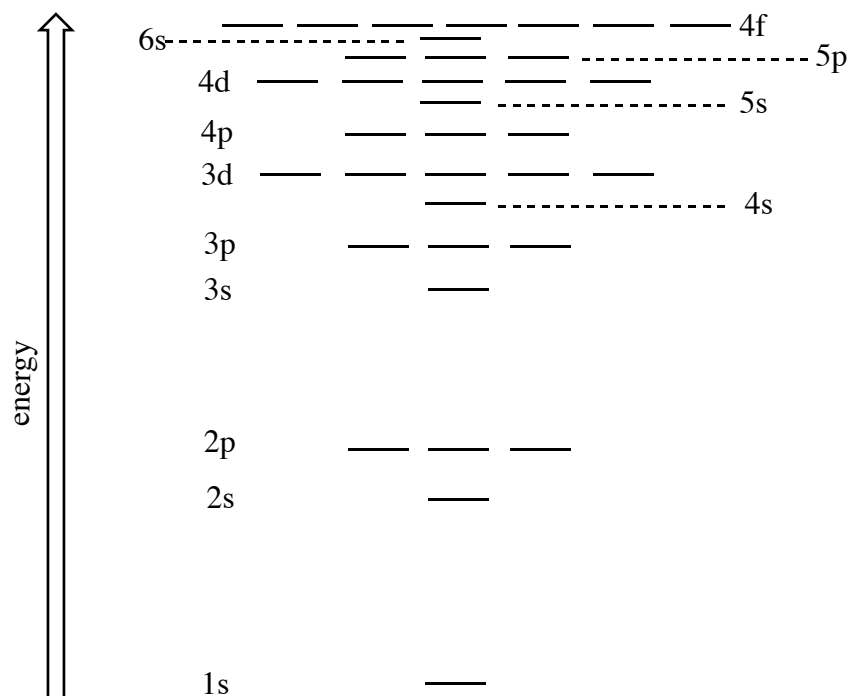
2<sup>nd</sup> shell:

3<sup>rd</sup> shell:

4<sup>th</sup> shell:

- By filling the orbitals with electrons, we arrive at the electronic configuration of any atom in the periodic table:

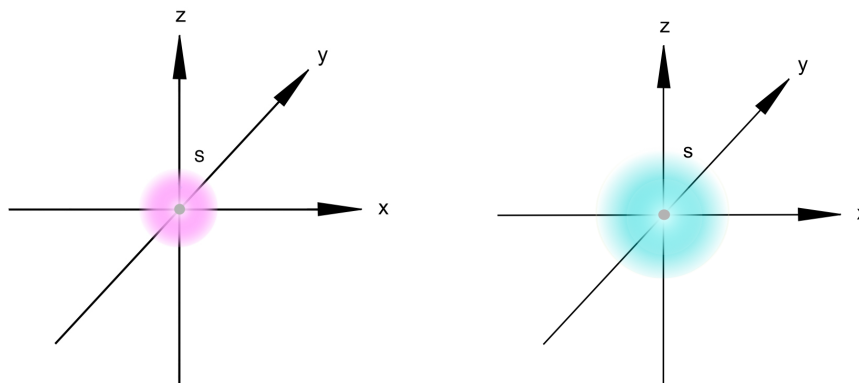
## Example: Carbon

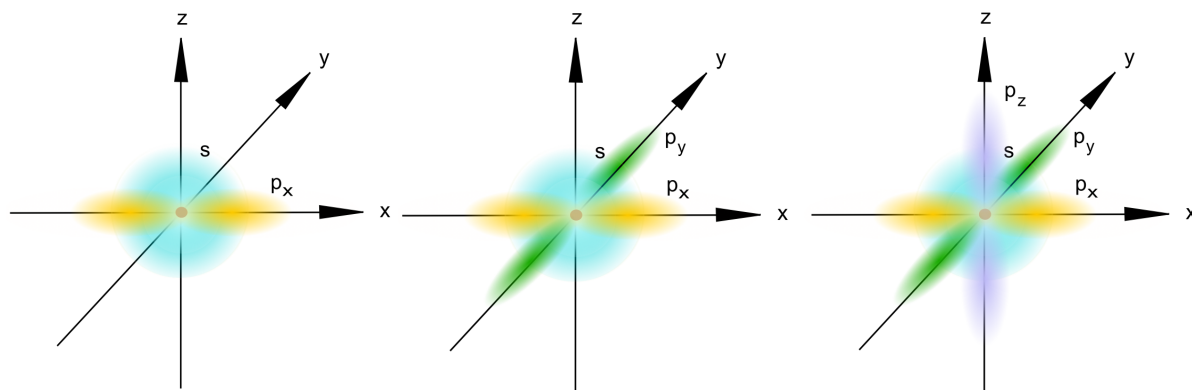


- lowest energy filled first (**Aufbau Principle**)
- maximum of 2 electrons per orbital with paired spins (**Pauli Exclusion Principle**)
- degenerate orbitals are filled with one electron each before electrons are paired (**Hund's Rule**)

## B. Atomic Orbitals

As we said previously, the square of the wave function ( $\Psi^2$ ) gives the probability of finding the electron at a given distance and direction from the nucleus. Plots of  $\Psi^2$  in three dimensions generate the shapes of s, p, d & f atomic orbitals.

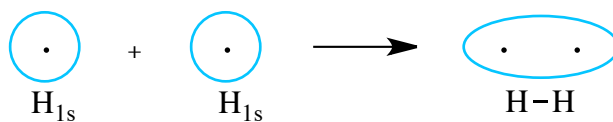




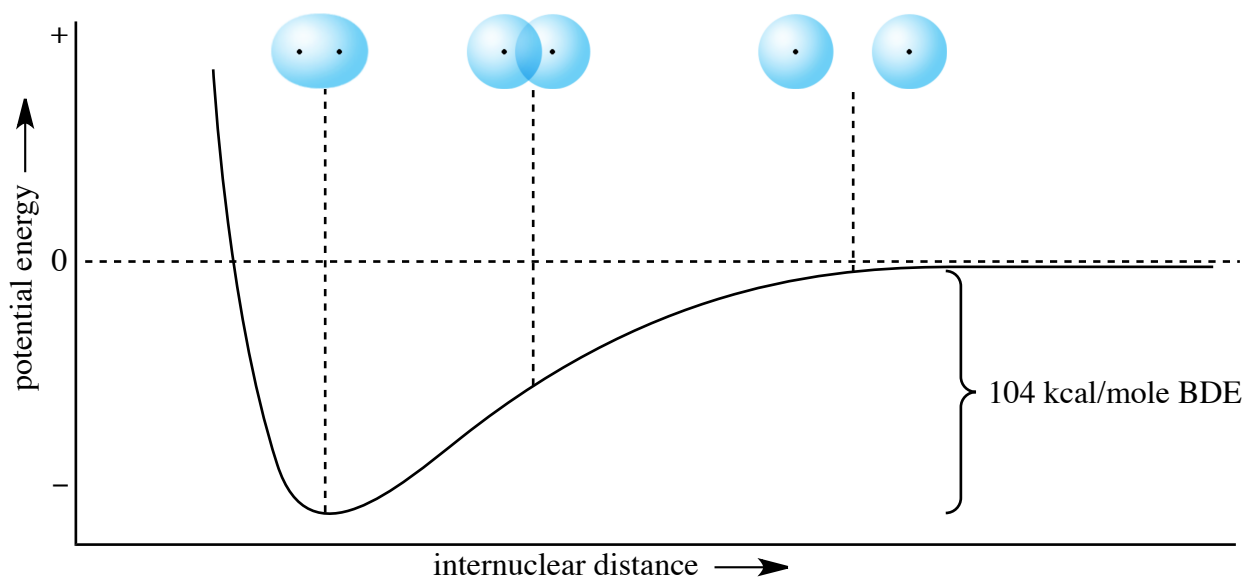
### C. Molecular Orbitals

Covalent bonds result from the combination of atomic orbitals to form molecular orbitals. A molecular orbital describes the volume in space around a molecule where an electron is likely to be found.

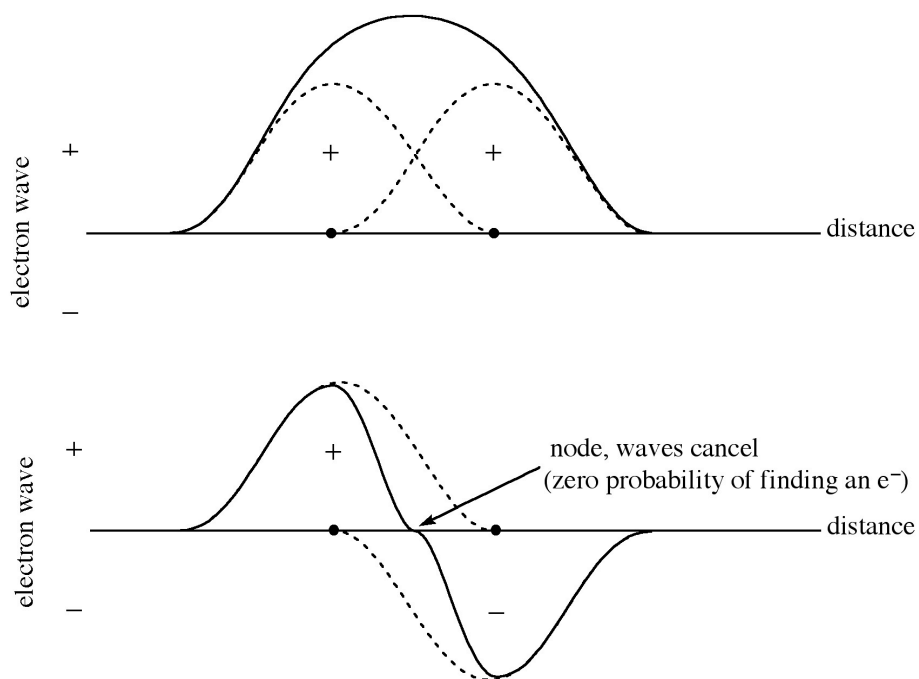
**Look** at the bonding in a hydrogen molecule, ( $H_2$ ):



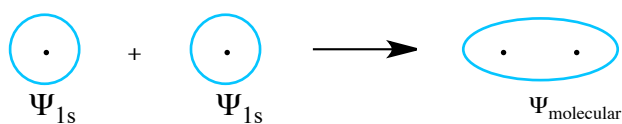
During bond formation, energy is released as the two orbitals start to overlap:



Phase is important when you add together wave functions:

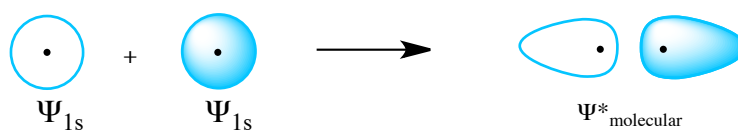


If two H atoms of the *same* phase are brought together:

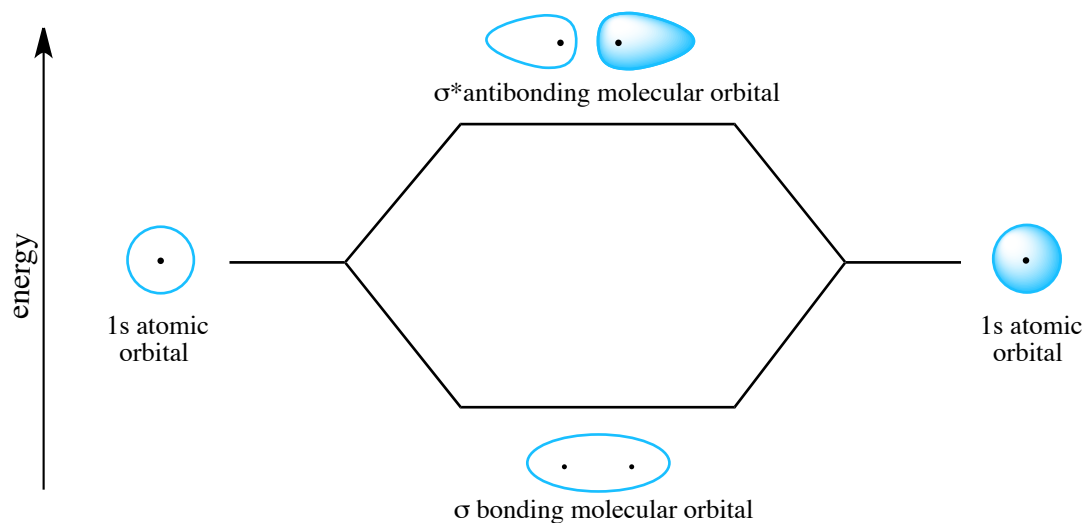


**$\sigma$ -bond:** concentrates electron density on the axis that joins two nuclei. A  $\sigma$ -bond has circular symmetry about the line connecting two nuclei.

If two H atoms of *opposite* phase are brought together:



The energy of the two possible combinations can be plotted:



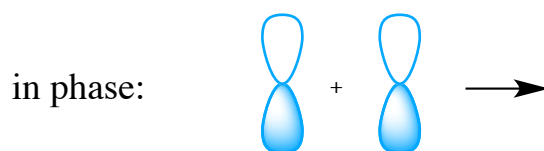
- A hydrogen molecule is more stable than two separate hydrogen atoms by about 104 kcal/mole.

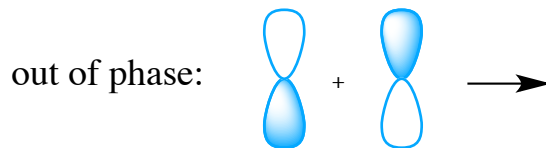
**p-orbitals can overlap end-on or sideways:**

*end on* overlap of *p*-orbitals creates a  **$\sigma$ -bond**:



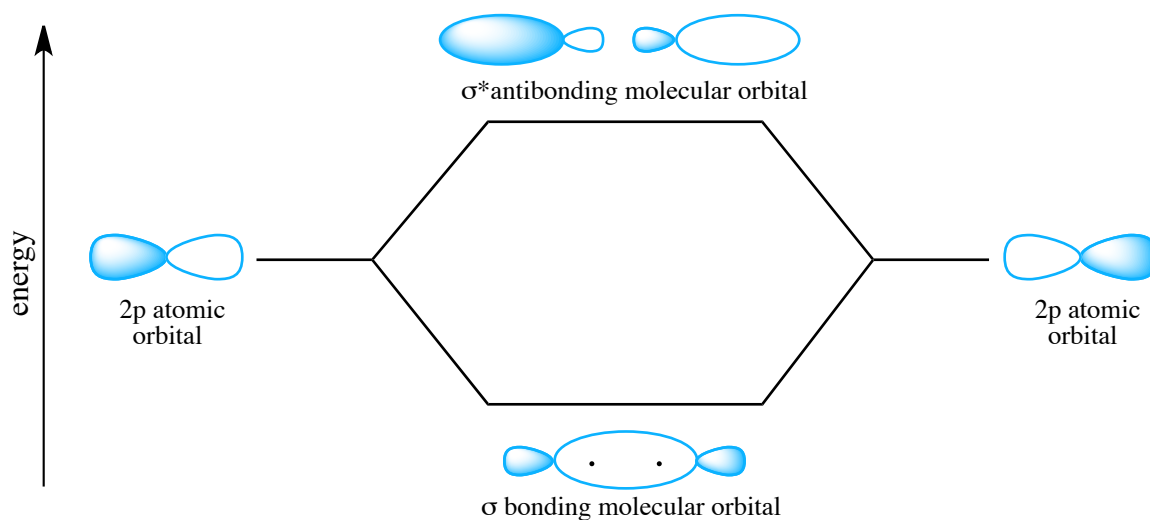
*sideways* overlap of *p*-orbitals creates a  **$\pi$ -bond**:



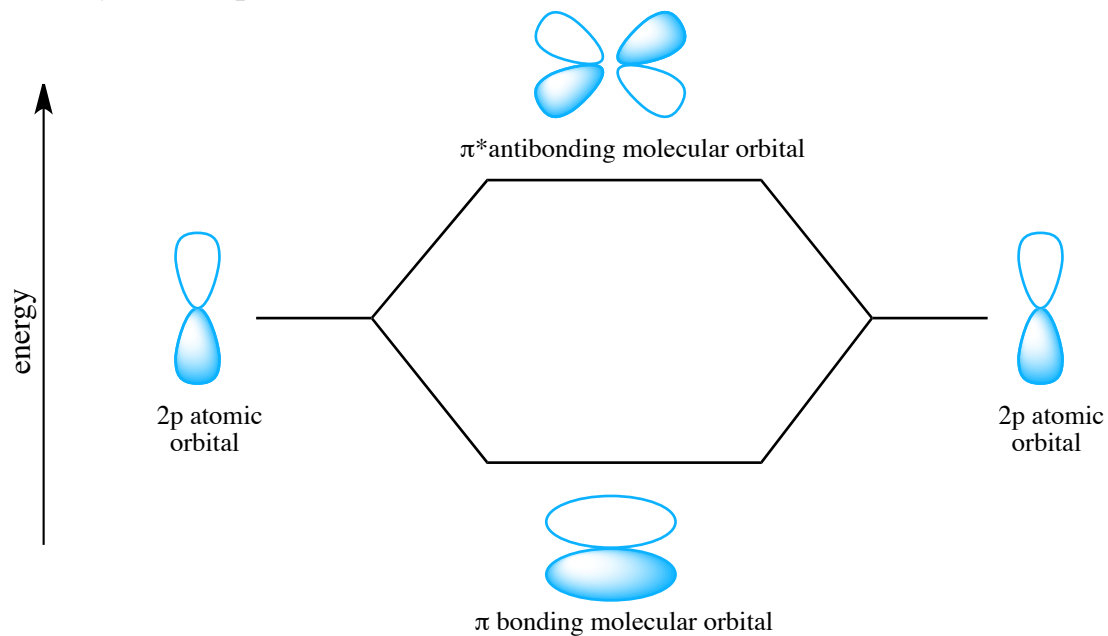


The energy of both of these combinations can be plotted:

*end on* overlap:



*sideways* overlap:



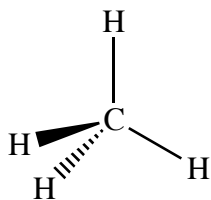


The extent of overlap is greater when  $p$ -orbitals overlap *end-on* than when they overlap *sideways*.

Result:

### D. Bonding in Methane

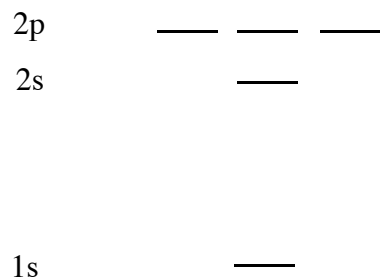
Using VSEPR, we predicted that methane is a tetrahedral molecule with 4 identical C-H bonds and bond angles of  $109.5^\circ$ . This is exactly what is experimentally observed for  $\text{CH}_4$ .



*How* do we describe the bonding in methane?

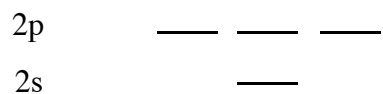
#### Problem #1:

We know carbon forms 4 bonds, but in the ground state electron configuration of carbon, there are only 2 unpaired electrons:



**Solution:** *Promote an Electron*

If an electron is promoted from the  $s$ -orbital to the empty  $p$ -orbital, carbon will now have 4 unpaired electrons, and can therefore make 4 bonds:



*energy cost to promote an electron:*

*energy released when 4 covalent bonds are made:*

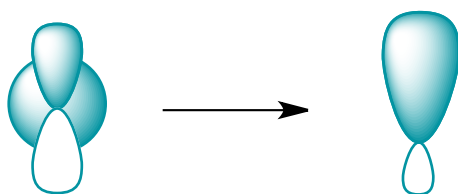
**net energy:**

*If only two covalent bonds are formed:*

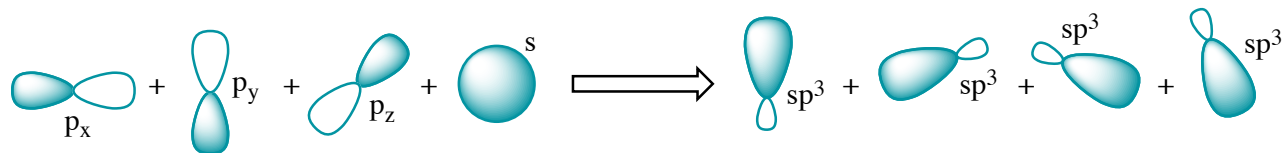
**Problem #2:**

Using  $s$  &  $p$  orbitals for bonding does not account for the structure of methane!

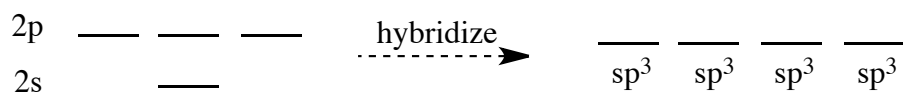
**Solution:** *Hybridize*



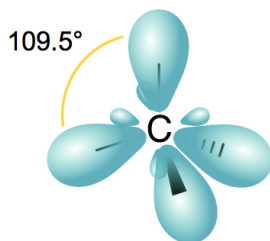
Combining three  $p$ -orbitals and one  $s$ -orbital gives four  $sp^3$  orbitals:



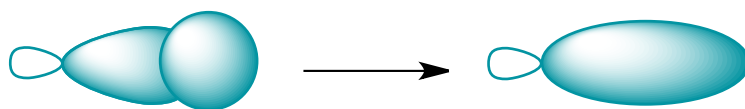
Energy levels:



All four  $sp^3$  orbitals superimposed:

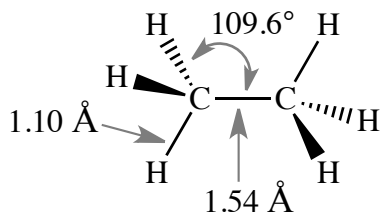


Each C-H both in Methane:

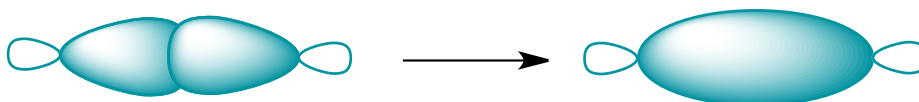


## D. Bonding in Ethane

Both carbons in ethane are tetrahedral:

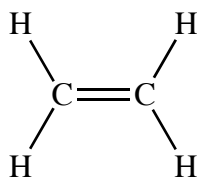


The C-C bond in ethane:



## E. Bonding in Ethylene: A Double Bond

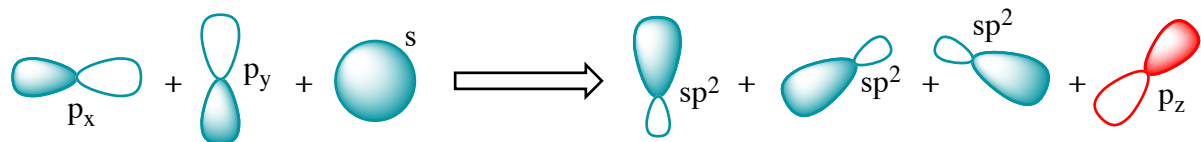
Using VSEPR, we predicted that ethylene is a trigonal planar molecule with 4 identical C-H bonds and bond angles of 120°. This is exactly what is experimentally observed for ethylene.



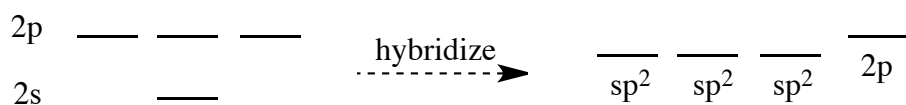
**How** do we describe the bonding in ethylene? Using **s** & **p** orbitals for bonding does not account for the structure of ethylene!

**Solution:** *Hybridize*

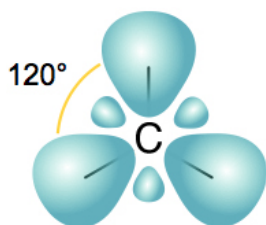
For carbon to bond to three atoms, we need to combine two *p*-orbitals and one *s*-orbital to give three *sp*<sup>2</sup> orbitals. One *p*-orbital remains unhybridized:



Energy levels:



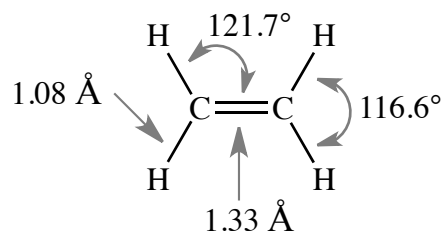
All three  $sp^2$  orbitals superimposed:



Bonding in ethylene:

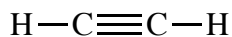
Notice: A double bond consists of a  $\sigma$ -bond and a  $\pi$ -bond!

Look at the bond lengths and bond angles in ethylene. What else do you notice?



## F. Bonding in Acetylene: A Triple Bond

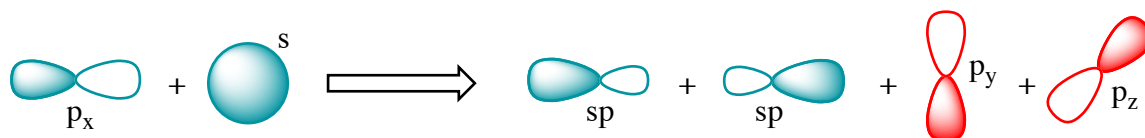
Using VSEPR, we predicted that acetylene is a linear molecule with 2 identical C-H bonds and bond angles of  $180^\circ$ . This is exactly what is experimentally observed for acetylene.



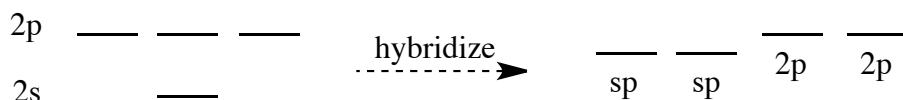
**How** do we describe the bonding in acetylene? Bond angles are consistent with the use of *s* & *p* orbitals for bonding, but experimentally the properties of acetylene are not consistent.

**Solution:** *Hybridize*

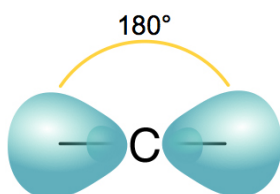
For carbon to bond to two atoms, we need to combine one *p*-orbital and one *s*-orbital to give two *sp* orbitals. Two *p*-orbitals remain unhybridized:



Energy levels:



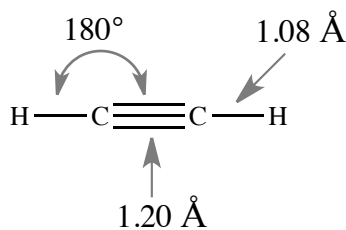
Both sp orbitals superimposed:



Bonding in acetylene:

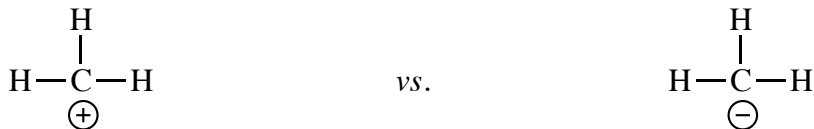
Notice: A triple bond consists of one  $\sigma$ -bond and two  $\pi$ -bonds!

*Look also at the bond lengths and bond angles in acetylene. What else do you notice?*



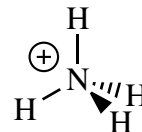
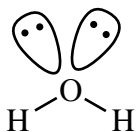
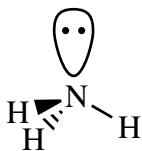
### G. Bonding in a Methyl Cation and a Methyl Anion

Using VSEPR, we can predict the geometry of a methyl cation, & a methyl anion, and describe the bonding.



### H. Bonding in a Ammonia, Water, and Ammonium ion

We can now describe the bonding in ammonia, water & ammonium ion:





Notice: The number of groups (*atoms & non-bonding electrons*) corresponds to the # of atomic orbitals that must be hybridized to form the hybrid orbitals:

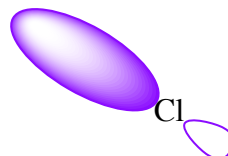
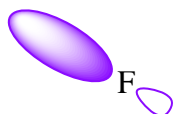
number of groups around atom	number of orbitals used	type of hybrid orbital
2	2	two sp orbitals
3	3	three sp <sup>2</sup> orbitals
4	4	four sp <sup>3</sup> orbitals

### I. Bonding in Hydrogen Halides

sp<sup>3</sup> hybridization also can be used to describe the bonding in hydrogen halides.

Look at H— $\overset{\cdot\cdot}{\underset{\cdot\cdot}{\text{F}}}$ :

*Compare* bonding in HF and in HCl:



## Hydrogen Halide Bond Lengths and Bond Strengths:

Hydrogen Halide	Bond length (Å)	Bond strength (kcal/mole)
H—F	0.917	136
H—Cl	1.2746	103
H—Br	1.4145	87
H—I	1.6090	71

This result can be generalized: Bond length *increases* and bond strength *decreases* with increasing atomic size as you descend any column in the periodic table.

**Q.** What happens across a row (period) in the periodic table?

**A.**

	H—C	H—N	H—O	H—F
<b>Bond length</b> (Å)	1.091	1.008	0.958	0.917
<b>Bond strength</b> (kcal/mole)	105	107	119	136

Notice: The change is not as dramatic as you move across a row.

Why?

## J. Relative Bond Length and Bond Strength of the Bonds in Ethane, Ethylene, and Acetylene

Important trends can be seen in the bond length and bond strength of the C-C and C-H bonds in ethane, ethylene and acetylene.

LOOK at the following chart:

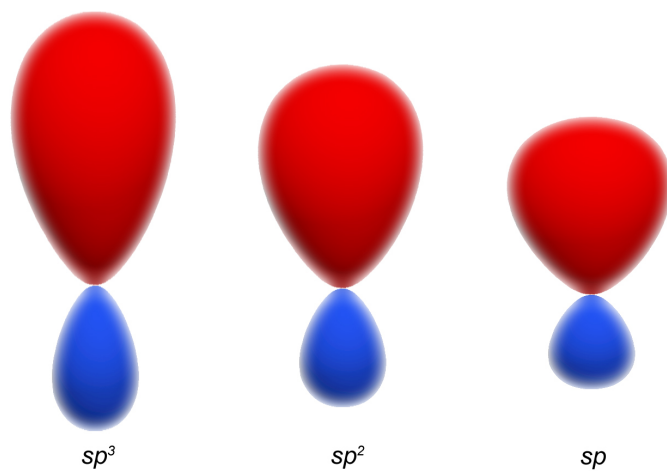
Molecule	Hybridization of carbon	Bond angles	Length of C-C bond (Å)	Strength of C-C bond (kcal/mole)	Length of C-H bond (Å)	Strength of C-H bond (kcal/mole)
$\begin{array}{c} \text{H} \quad \text{H} \\   \quad   \\ \text{H}-\text{C}-\text{C}-\text{H} \\   \quad   \\ \text{H} \quad \text{H} \end{array}$	sp <sup>3</sup>	109.5°	1.54	90	1.10	101
$\begin{array}{c} \text{H} \quad \quad \text{H} \\ \diagdown \quad / \\ \text{C}=\text{C} \\ / \quad \diagdown \\ \text{H} \quad \quad \text{H} \end{array}$	sp <sup>2</sup>	120°	1.33	174	1.08	111
H—C≡C—H	sp	180°	1.20	231	1.06	131

**Important points:**

- A double bond ( $\sigma + \pi$ ) is stronger than a single bond, but not twice as strong.
- The more “s” character a hybrid orbital has, the closer to the nucleus, and the more tightly held are its electrons



Compare an  $sp$ ,  $sp^2$ , and  $sp^3$  orbital:



- The length and strength of a C—H bond depends on the hybridization of the carbon atom it is attached to.
- A C—H  $\sigma$ -bond is shorter and stronger than a C—C  $\sigma$ -bond!
- The greater the  $s$ -character in the orbital, the larger the bond angle.

## VI. Electronegativity and Bond Polarity

***nonpolar covalent bond:***                      bonding electrons shared equally (both atoms have the same electronegativity)

**polar covalent bond:** bonding electrons are shared unequally (two atoms with different electronegativities)

$\delta+$ : the atom is electron deficient (has a partial positive charge)

$\delta-$  : the atom is electron rich (has a partial negative charge)

higher electronegativity = greater attraction for electrons

The greater the difference in electronegativity, the greater the polarity of the bond:

Na & Cl

C & H

H-O C-Hal

H-F C-O

H-Cl C-N H-N

☞ **Recall:** If electronegativity difference is greater than about 1.8, the electron will be transferred completely and you will have an ionic bond

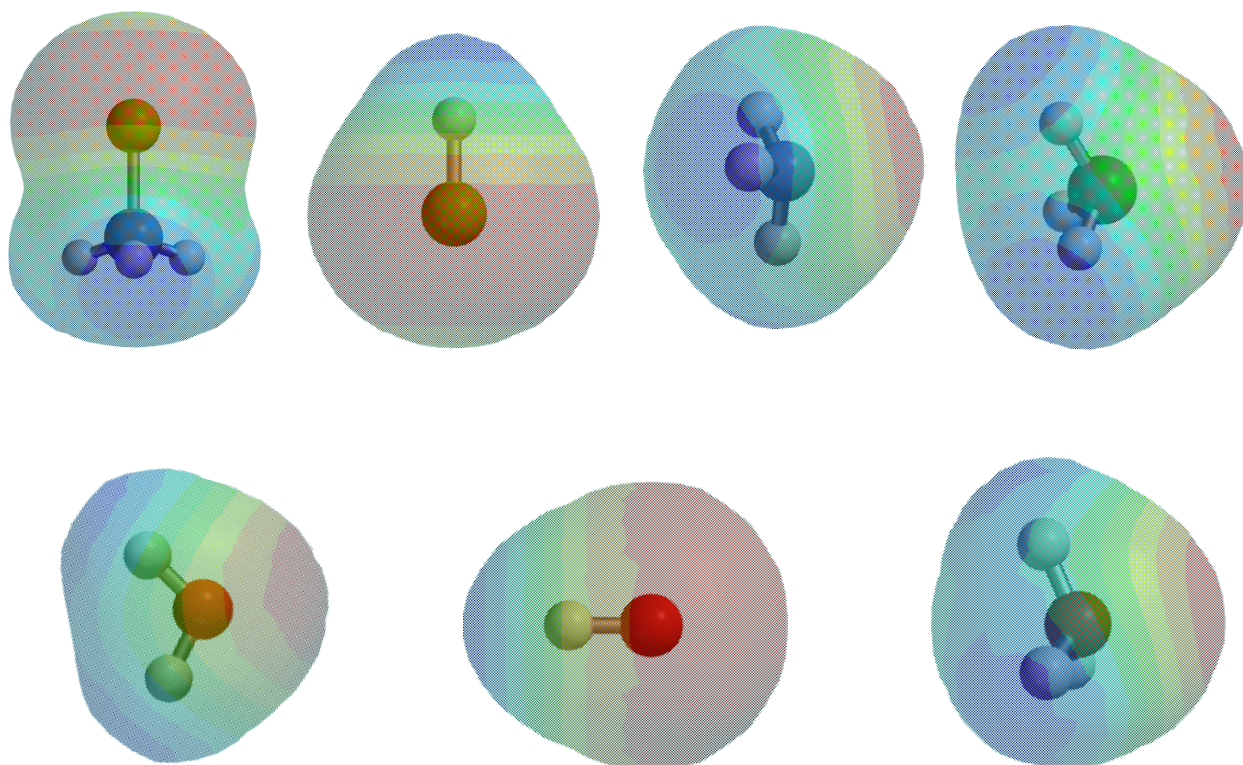
Understanding bond polarity is **critical** to your understanding of organic chemistry!

**Electrostatic potential maps** are very helpful in showing how the charge is distributed in a molecule (*see page 44, 3<sup>rd</sup> ed. or 46, 4<sup>th</sup> ed.*). The colors on a potential map indicate the degree to which a molecule or an atom in a molecule attracts charged particles. The colors can also be used to estimate charge distribution.

red < orange < yellow < green < blue



**Examples:**



A polar bond has a dipole – it has a negative end and a positive end. The size of the dipole is indicated by the **dipole moment,  $\mu$** .

$$\text{dipole moment} = \mu = e \times d$$

LOOK at the following chart of bond dipole moments:

<b>Bond</b>	<b>Dipole moment, <math>\mu</math></b>	<b>Bond</b>	<b>Dipole moment, <math>\mu</math></b>
C—N	0.22 D	H—C	0.3 D
C—O	0.86 D	H—N	1.31 D
C—F	1.51 D	H—O	1.53 D
C—Cl	1.56 D	C=O	2.4 D
C—Br	1.48 D	C $\equiv$ N	3.6 D
C—I	1.29 D		

Some things you should notice:

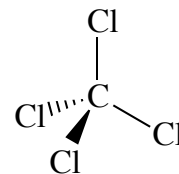
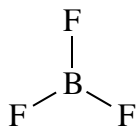
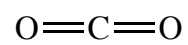
In a molecule with only one covalent bond, the dipole moment of the molecule is identical to the dipole moment of the bond. The dipole moment of a molecule with more than one covalent bond depends on the dipole moments of all the covalent bonds in the molecule and the geometry of the molecule.

## VII. Polarity of Molecules

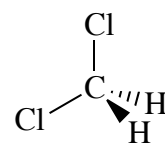
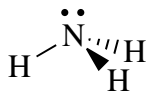
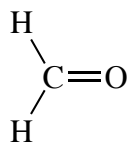
The dipole moment ( $\mu$ ) of a molecule is the vector sum of all the bond dipoles in the molecule. A vector has magnitude and direction, so the 3-D structure of the molecule must be taken into account. A molecule may contain polar bonds but have no overall dipole moment, depending on the geometry

### Examples:

Some nonpolar molecules that have polar bonds:



Some polar molecules:





## Attributions

### Pages 16-17: Atomic orbitals:

[http://commons.wikimedia.org/wiki/Category:Atomic\\_orbitals#mediaviewer/File:Orbitale\\_s\\_px\\_py\\_pz.svg](http://commons.wikimedia.org/wiki/Category:Atomic_orbitals#mediaviewer/File:Orbitale_s_px_py_pz.svg)

[http://commons.wikimedia.org/wiki/Category:Atomic\\_orbitals#mediaviewer/File:Orbitale\\_s\\_px\\_py.svg](http://commons.wikimedia.org/wiki/Category:Atomic_orbitals#mediaviewer/File:Orbitale_s_px_py.svg)

[http://commons.wikimedia.org/wiki/Category:Atomic\\_orbitals#mediaviewer/File:Orbitale\\_s\\_px.svg](http://commons.wikimedia.org/wiki/Category:Atomic_orbitals#mediaviewer/File:Orbitale_s_px.svg)

[http://commons.wikimedia.org/wiki/Category:Atomic\\_orbitals#mediaviewer/File:Orbitale\\_s.svg](http://commons.wikimedia.org/wiki/Category:Atomic_orbitals#mediaviewer/File:Orbitale_s.svg)

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### Page 23: $sp^3$ -hybridized carbon. Adapted from:

<http://upload.wikimedia.org/wikipedia/commons/a/a5/AE4h.svg>

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### Page 25: $sp^2$ -hybridized carbon. Adapted from:

<http://upload.wikimedia.org/wikipedia/commons/1/15/AE3h.svg>

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### Page 27: $sp$ -hybridized carbon. Adapted from:

<http://upload.wikimedia.org/wikipedia/commons/4/49/AE2h.svg>

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