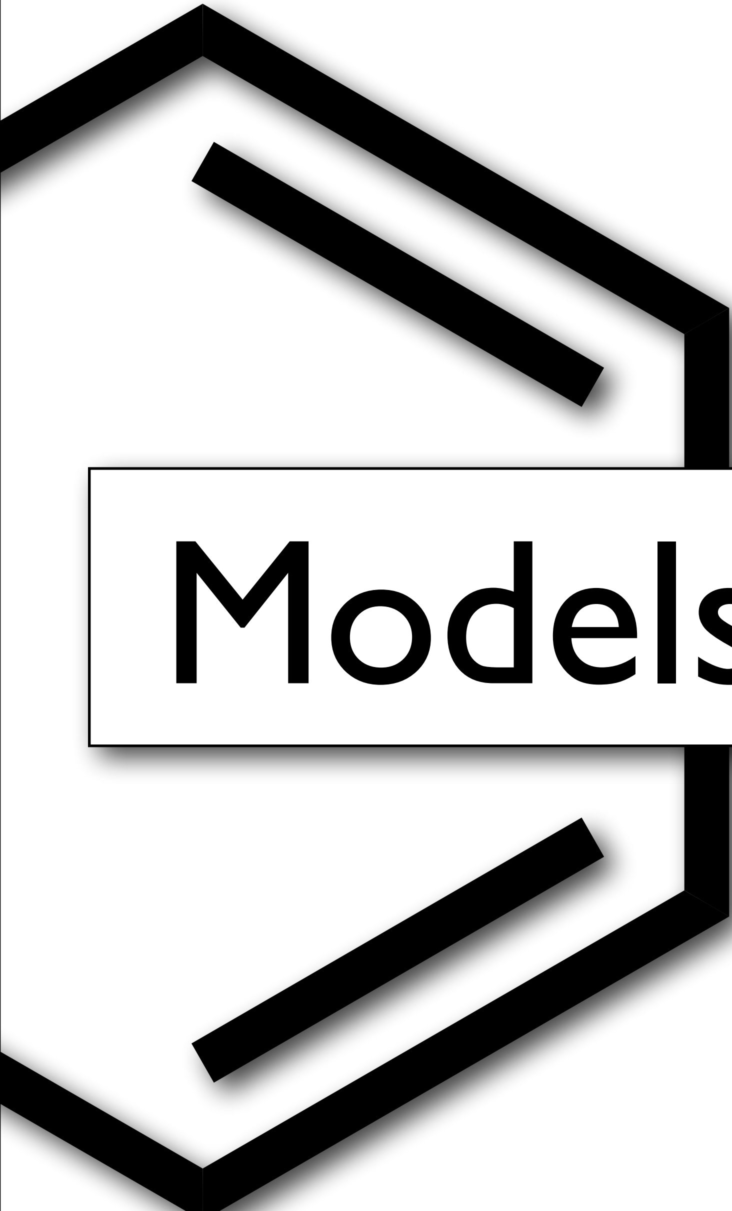
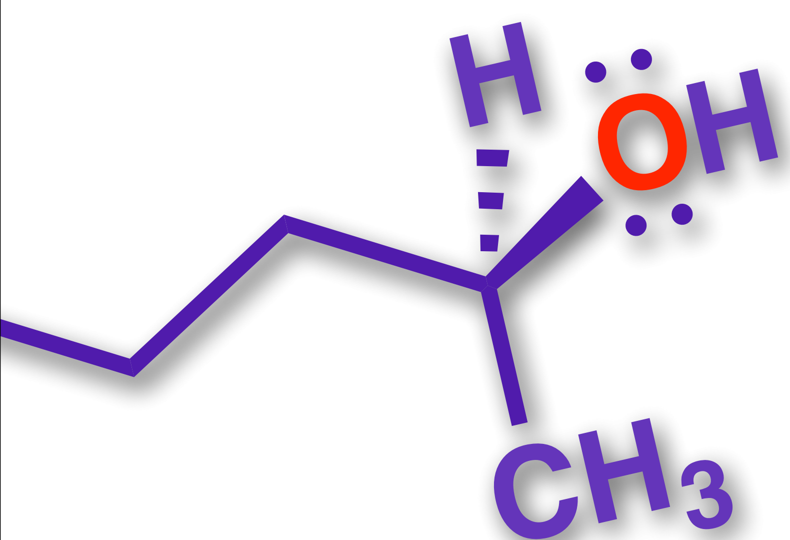


Models of Chemical Bonding



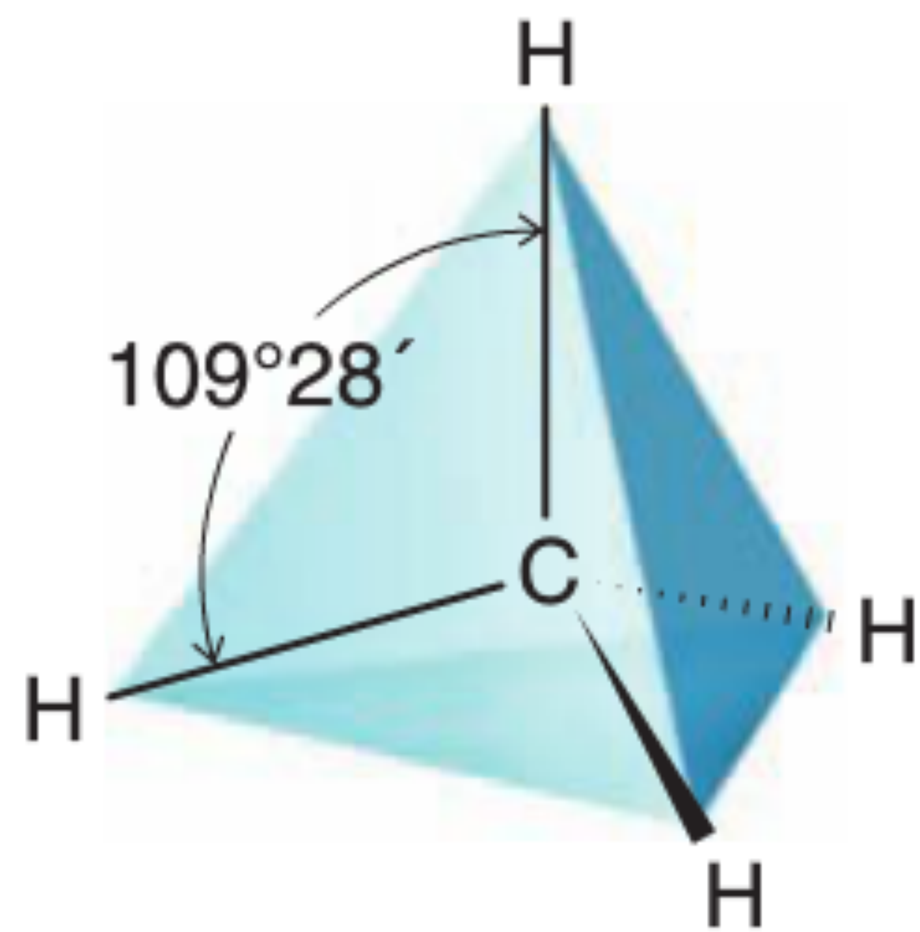
Chemistry Lecture 2

Outline II

- Three-Dimensional Formulas
- VSEPR Theory
- Polar Covalent Bonds
- Dipole Moments
- Structural Formulas- Condensed and Bond-Line

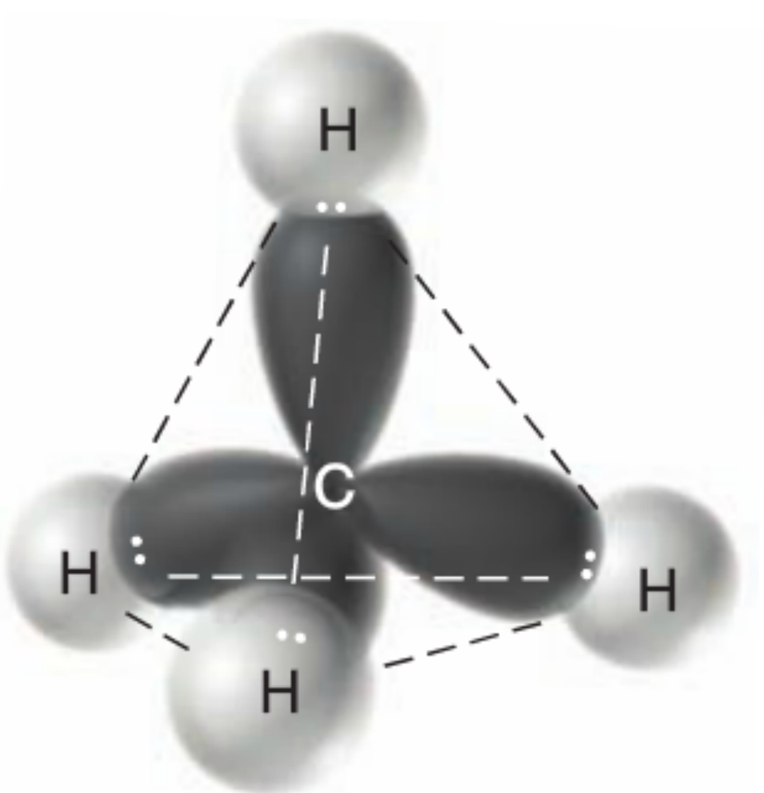
Molecular Shape

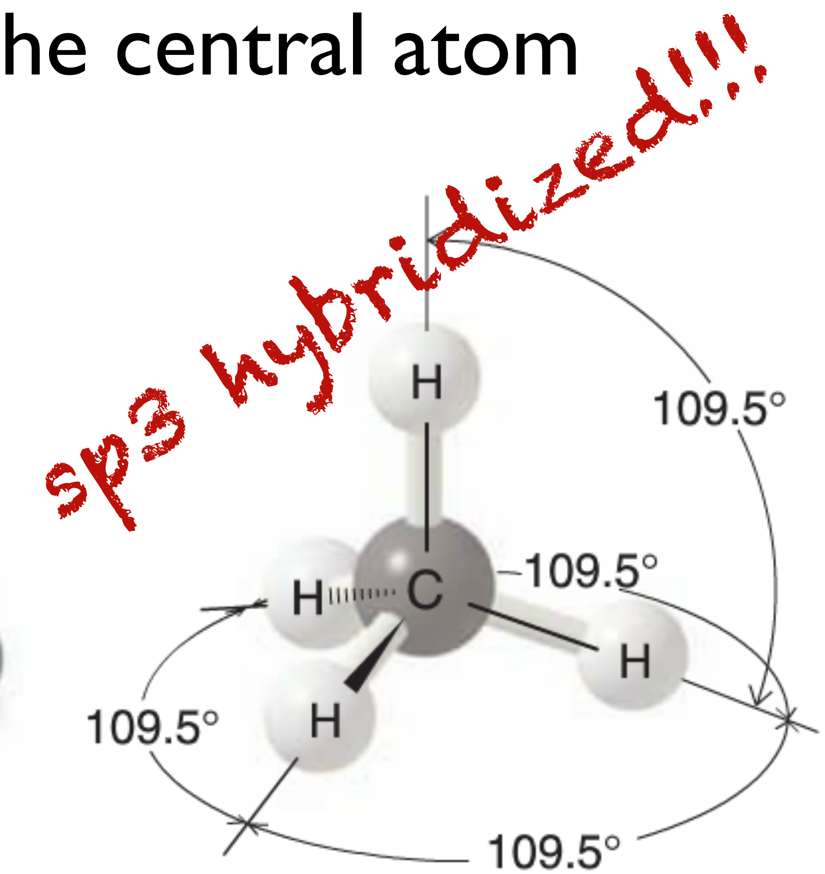
- Bond line formulas also better represent true molecular shape
- The bond angles in CH_4 are NOT 90° !!!!!!!
- They are ~109.5°



Valence Shell Electron Pair Repulsion Theory

- Considers the electrons in the valence shell around a central atom
- These electrons want to be as far apart from one another as possible
- In methane, the electrons adopt a tetrahedral arrangement with 109.5 degree angles
- The shape of the molecule is determined by the arrangement of atoms around the central atom

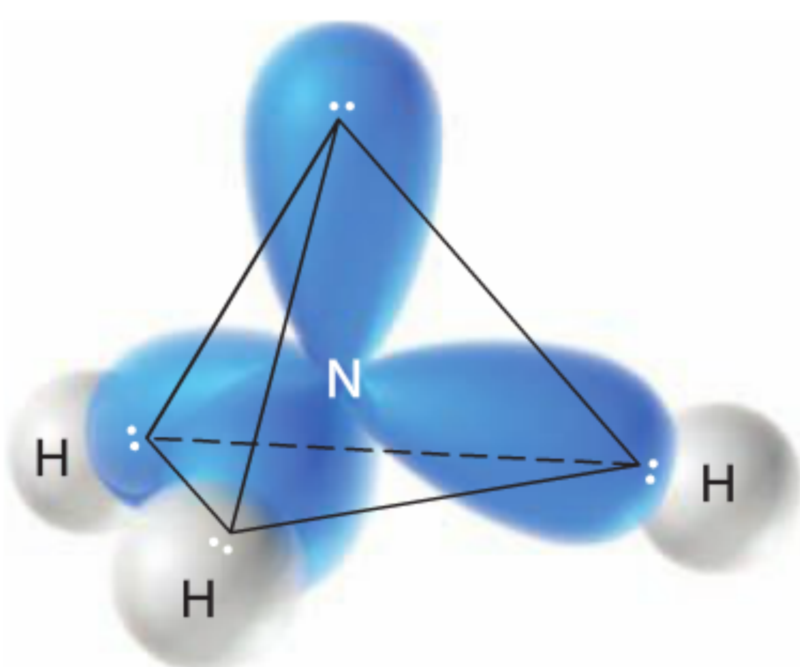


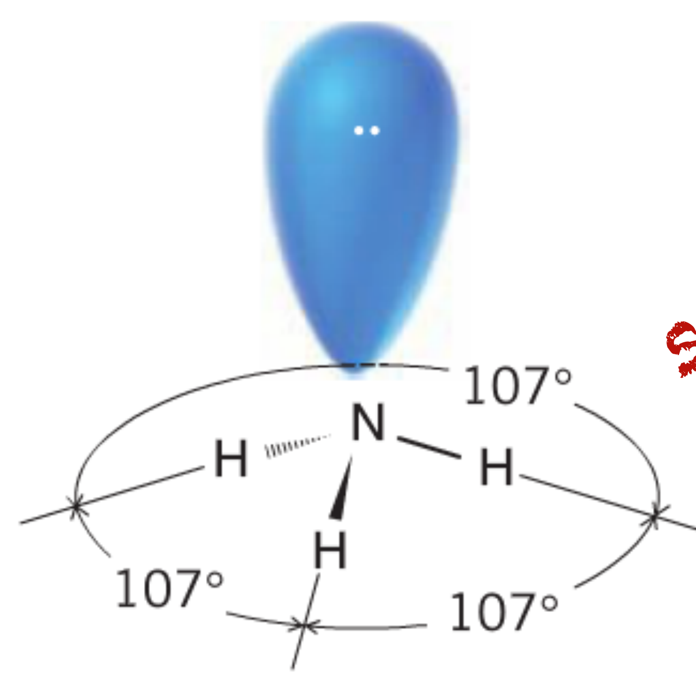


VSEPR Applications: Ammonia

- Ammonia has a lone pair and three bonds to Hs
- The electron geometry remains largely tetrahedral
- The molecular geometry is a trigonal pyramid
- But because the lp is not shared with another atom, these electrons take up more space than bonded e-
- The result is that the bond angles between the atoms attached to N are slightly smaller than 109.5 degrees

sp3 hybridized!!!

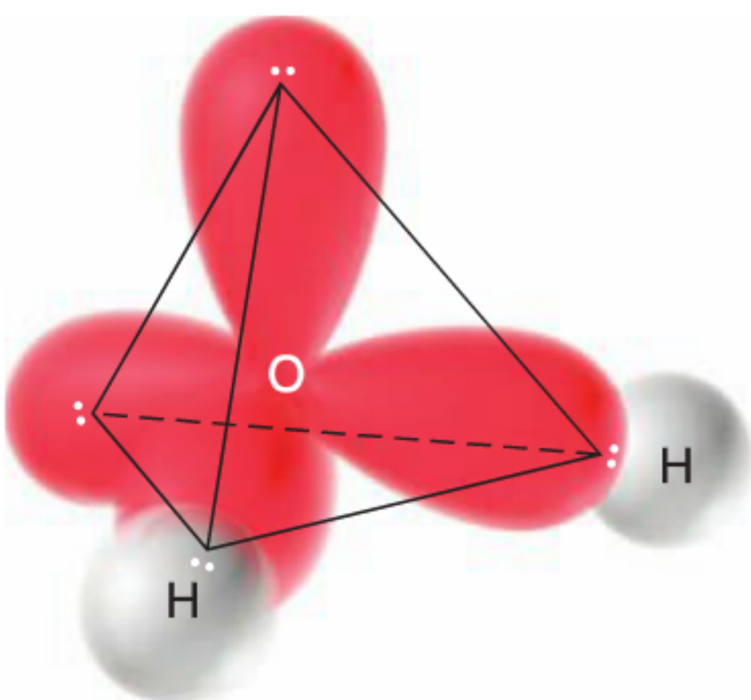


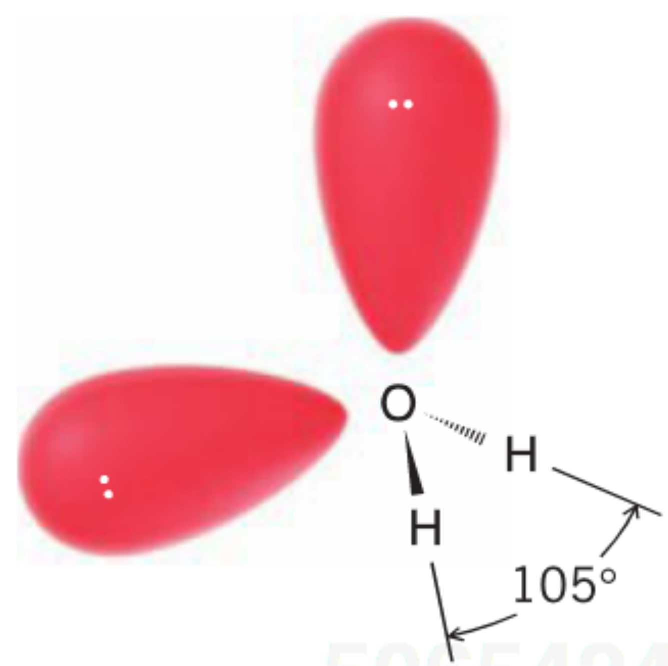


VSEPR Applications: Water

- Water has two lone pair and two bonds to Hs
- The electron geometry remains largely tetrahedral
- The molecular geometry is bent or angular
- But because the lp are not shared with other atoms, these electrons take up more space than bonded e-
- The result is that the bond angles between the atoms attached to O are much smaller than 109.5 degrees

sp3 hybridized!!!

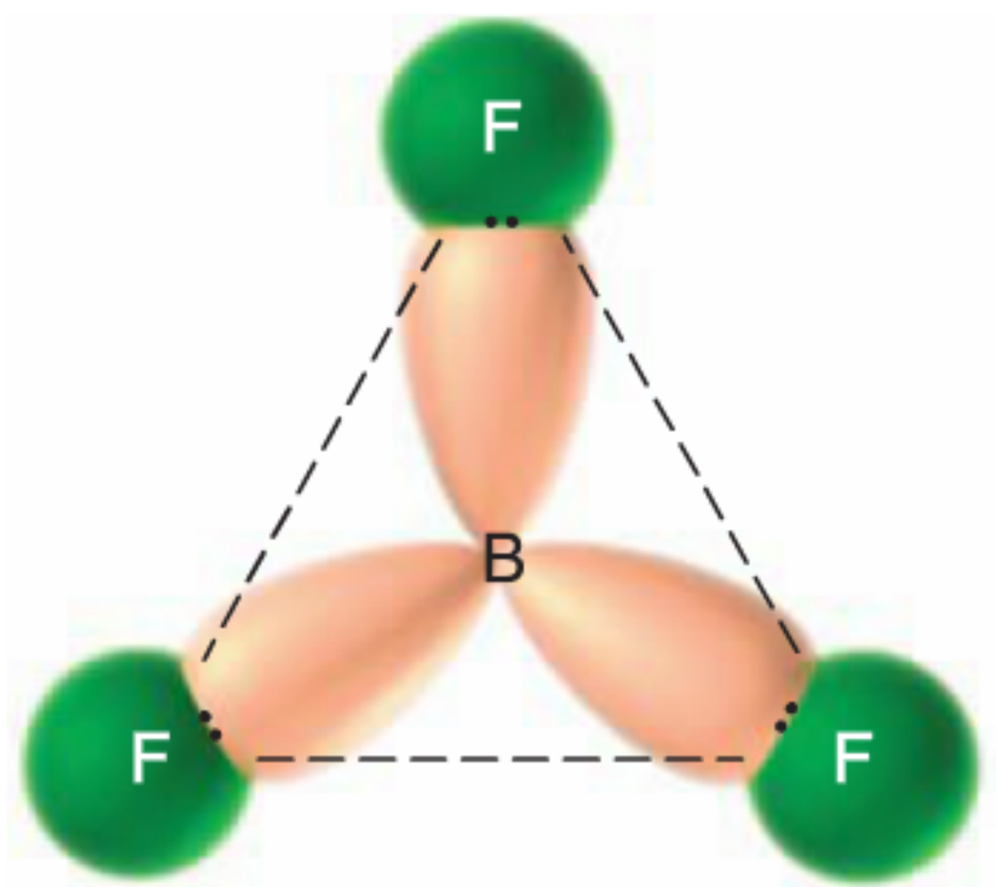


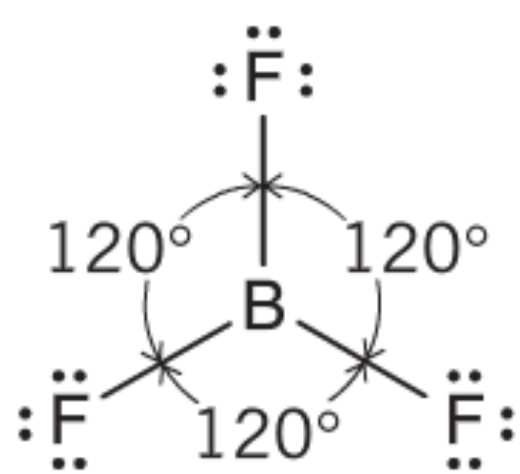


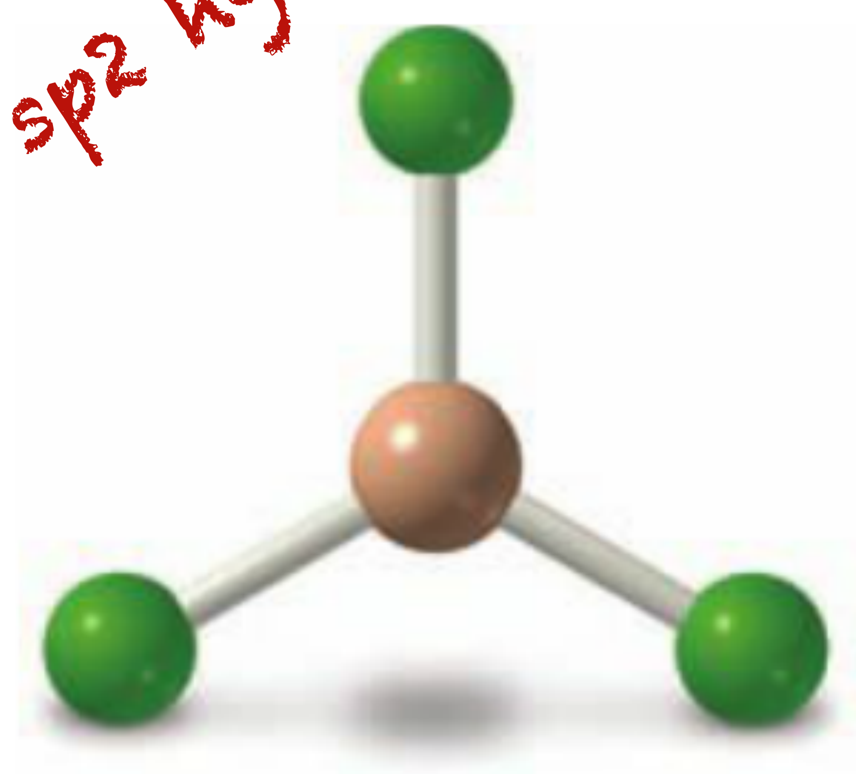
VSEPR Applications: BF_3

- BF_3 has no lone pairs and three bonds to Fs
- The electron geometry is trigonal
- The molecular geometry is a trigonal
- The lack of lp electrons allows BF_3 to adopt a flat shape

sp2 hybridized!!!

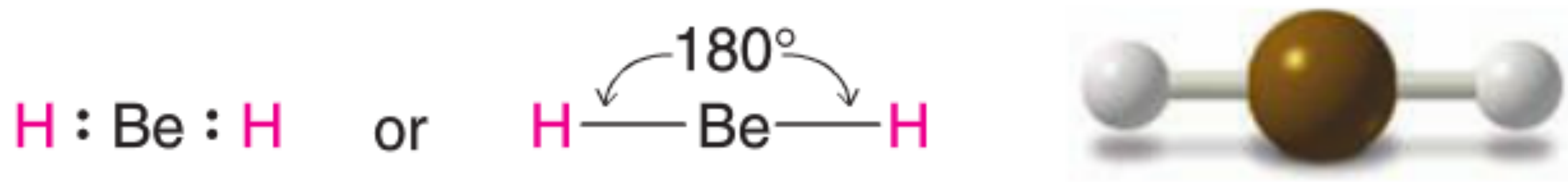






VSEPR Applications: BeH_2

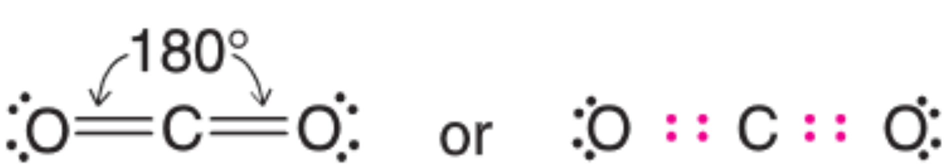
- BeH_2 has no lone pairs and two bonds to Hs
- The electron geometry is linear
- The molecular geometry is linear



Linear geometry of BeH_2

- Even if the bonds are double bonds, VSEPR theory still allows for the prediction of molecular shape
- CO_2 has a linear electron and molecular geometry

sp hybridized!!!



The four electrons of each double bond act as a single unit and are maximally separated from each other.

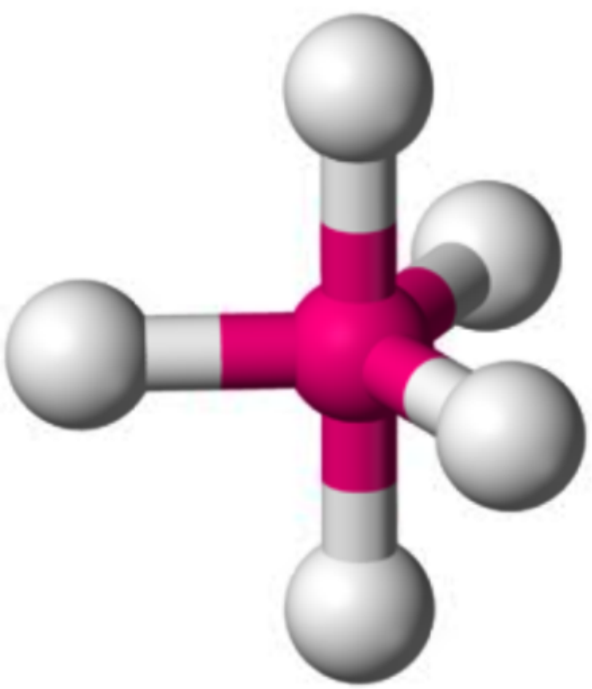
VSEPR for Simple Molecules

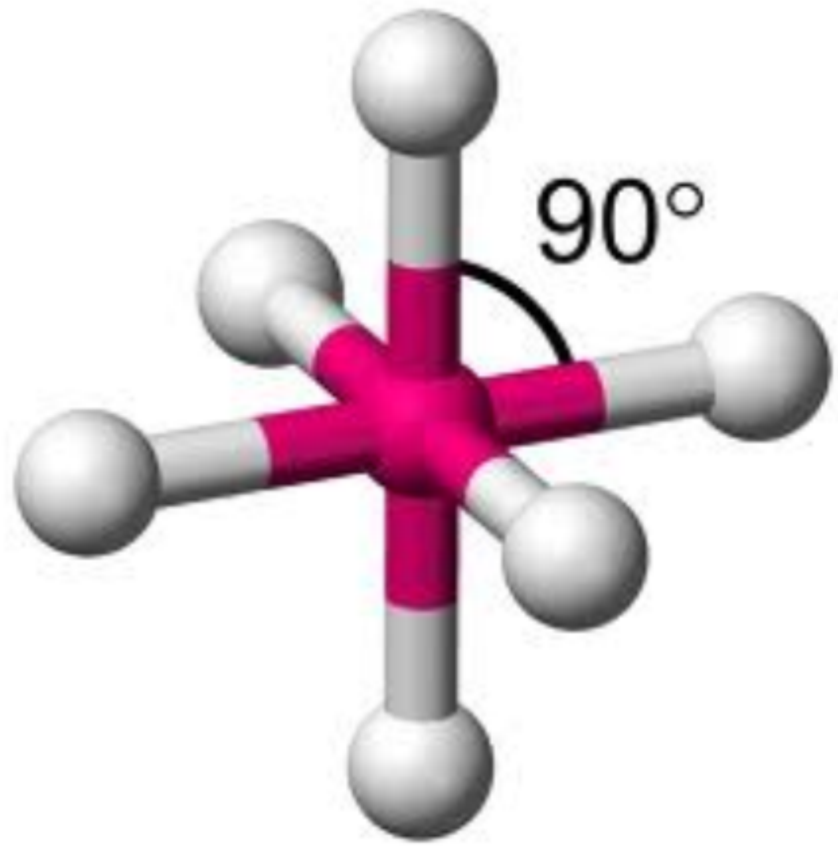
Number of Electron Pairs at Central Atom			Hybridization State of Central Atom	Shape of Molecule or Ion[a]	Examples
Bonding	Nonbonding	Total			
2	0	2	*sp*	Linear	BeH_2
3	0	3	sp^2	Trigonal planar	BF_3, $\overset{+}{C}H_3$
4	0	4	sp^3	Tetrahedral	CH_4, $\overset{+}{N}H_4$
3	1	4	$\sim sp^3$	Trigonal pyramidal	NH_3, $\overset{-}{C}H_3$
2	2	4	$\sim sp^3$	Angular	H_2O

[a]Referring to positions of atoms and excluding nonbonding pairs.

VSEPR for More Complex Molecules

- Atoms with greater than eight electrons in the valence shell can adopt more complex shapes
  - Trigonal bipyramidal, PCl5
  - Octahedral, SF6





- Let's arrive at these with examples: PCl5, SF6

VSEPR Examples

- H_2S
- PBr_3
- O_3
- H_2CO
- Cl_2C
- XeF_2
- HCN

Electronegativity

- Electronegativity - The measure of the ability of an atom to attract electrons
  - Trend apparent on the Periodic Table

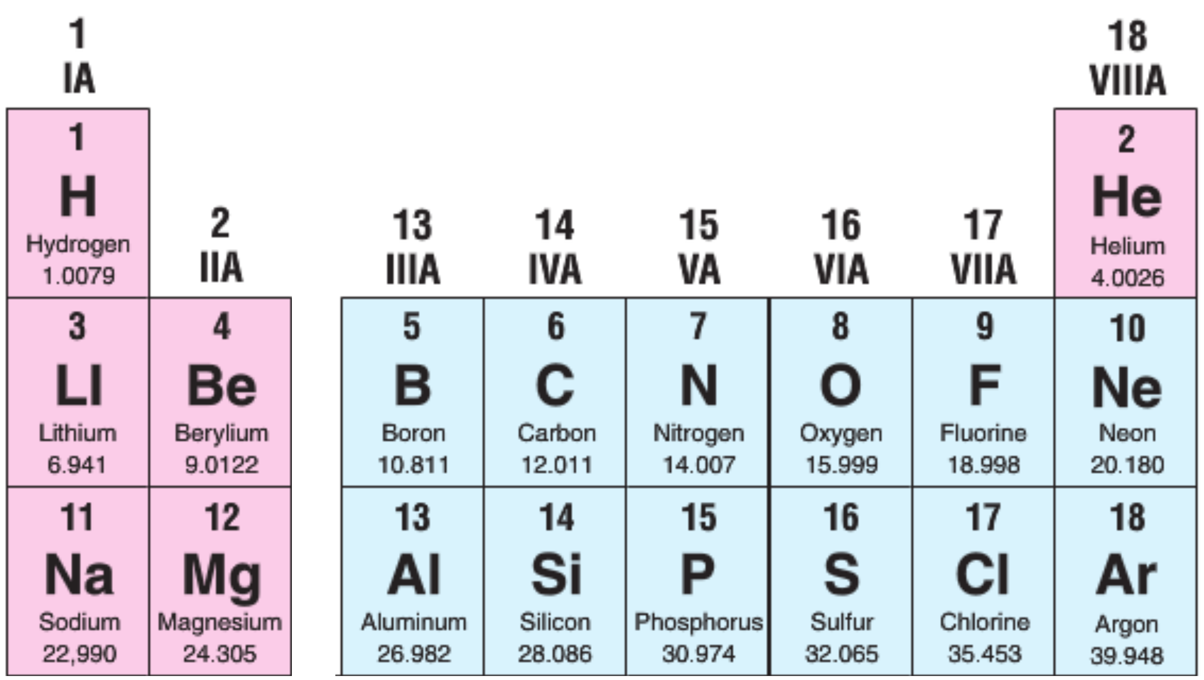


TABLE 1.1 ELECTRONEGATIVITIES OF SOME OF THE ELEMENTS

Increasing electronegativity →

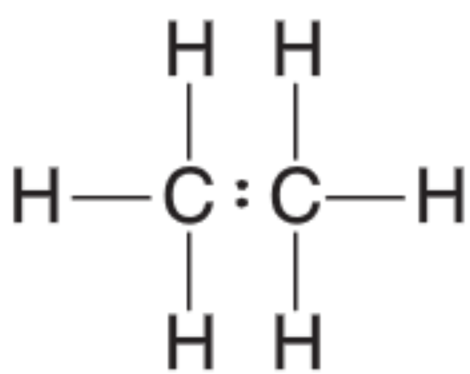
H 2.1

Li 1.0	Be 1.5	B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2	Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8						Br 2.8

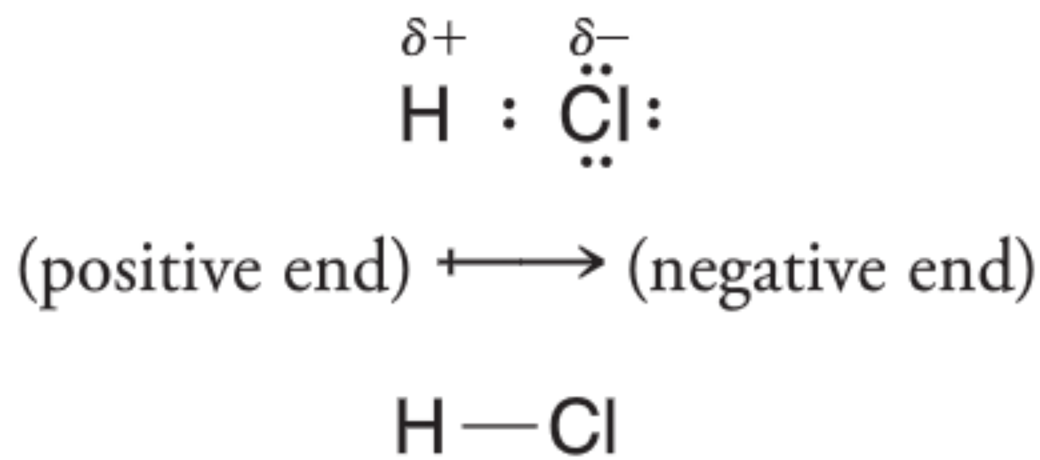
↑ Increasing electronegativity

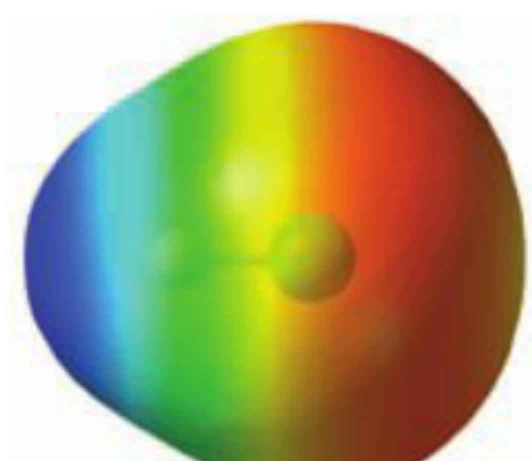
Polar Covalent Bonds

- Covalently bonded atoms with similar electronegativities share the two electrons equally
- Covalent bonds between atoms of different electronegativities have an unequal sharing of e-
- These are referred to as polar covalent bonds



Ethane has a covalent bond. The electrons are shared equally between the carbon atoms.





Dipole Moments

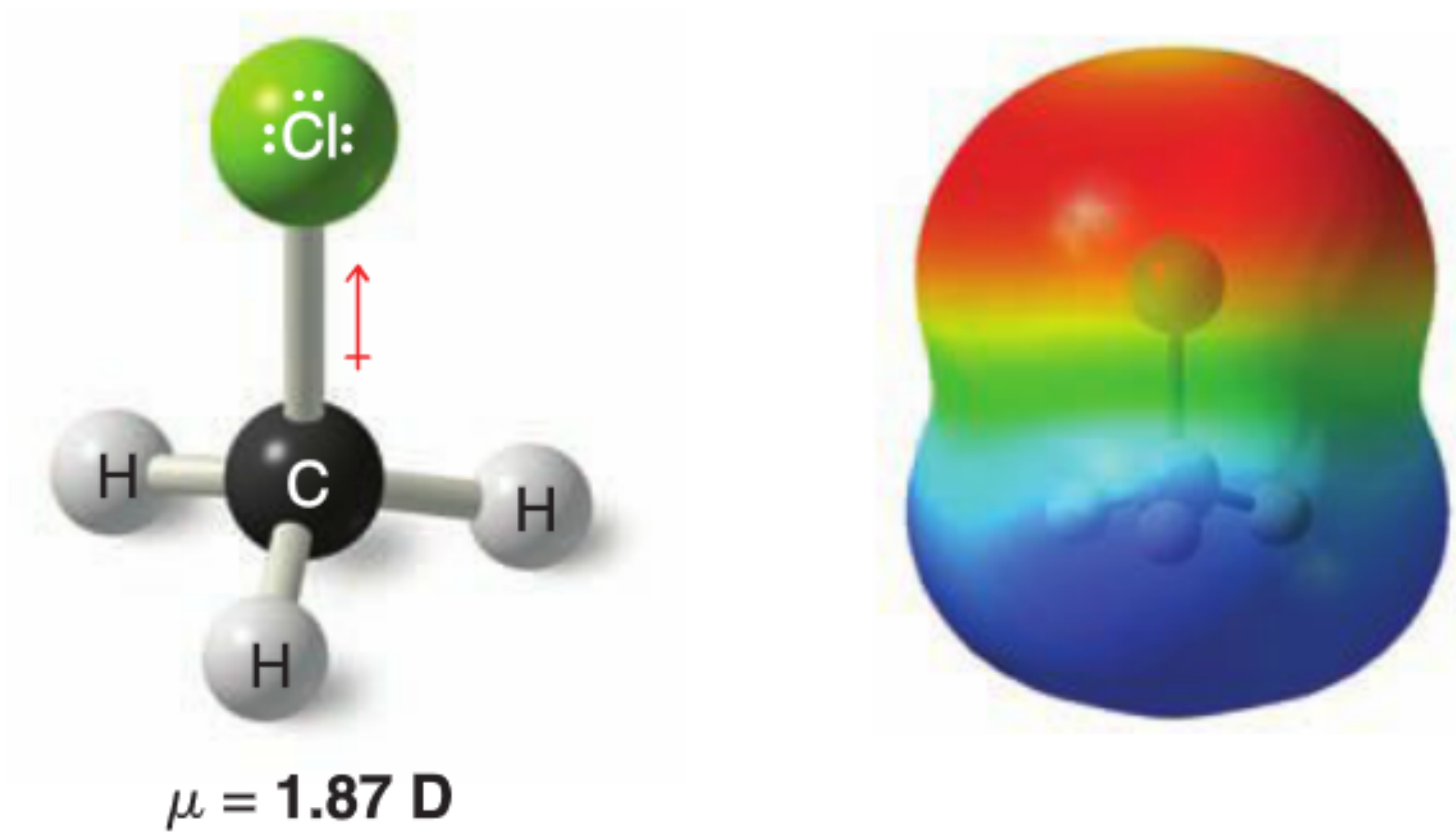
- The polarization in a bond or molecule is measure by a dipole moment
- A dipole moment is a measure of charge by distance
- A Debye (mu) is the unit of measure

TABLE 2.1 DIPOLE MOMENTS OF SOME SIMPLE MOLECULES

Formula	μ (D)	Formula	μ (D)
H_2	0	CH_4	0
Cl_2	0	CH_3Cl	1.87
HF	1.83	CH_2Cl_2	1.55
HCl	1.08	$CHCl_3$	1.02
HBr	0.80	CCl_4	0
HI	0.42	NH_3	1.47
BF_3	0	NF_3	0.24
CO_2	0	H_2O	1.85

Dipole Moments are Vectors

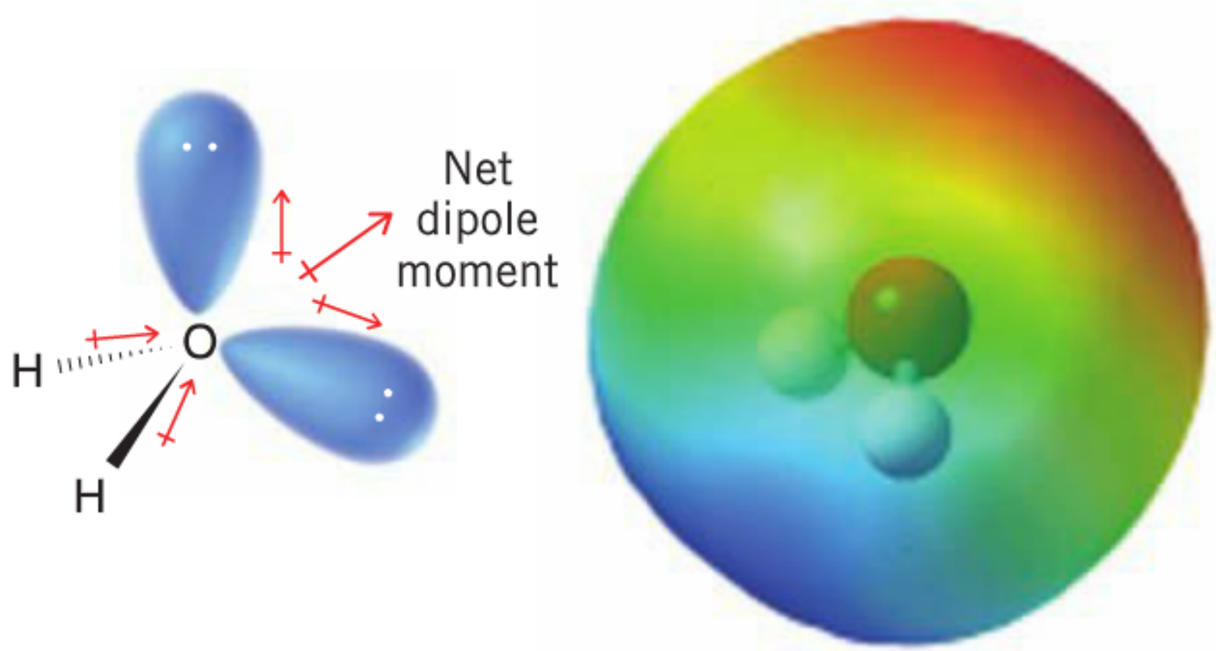
- Chloromethane has a very polarized C-Cl bond, whereas the C-H bonds are less polarized
- The overall polarization of the molecule is a pull toward the chlorine



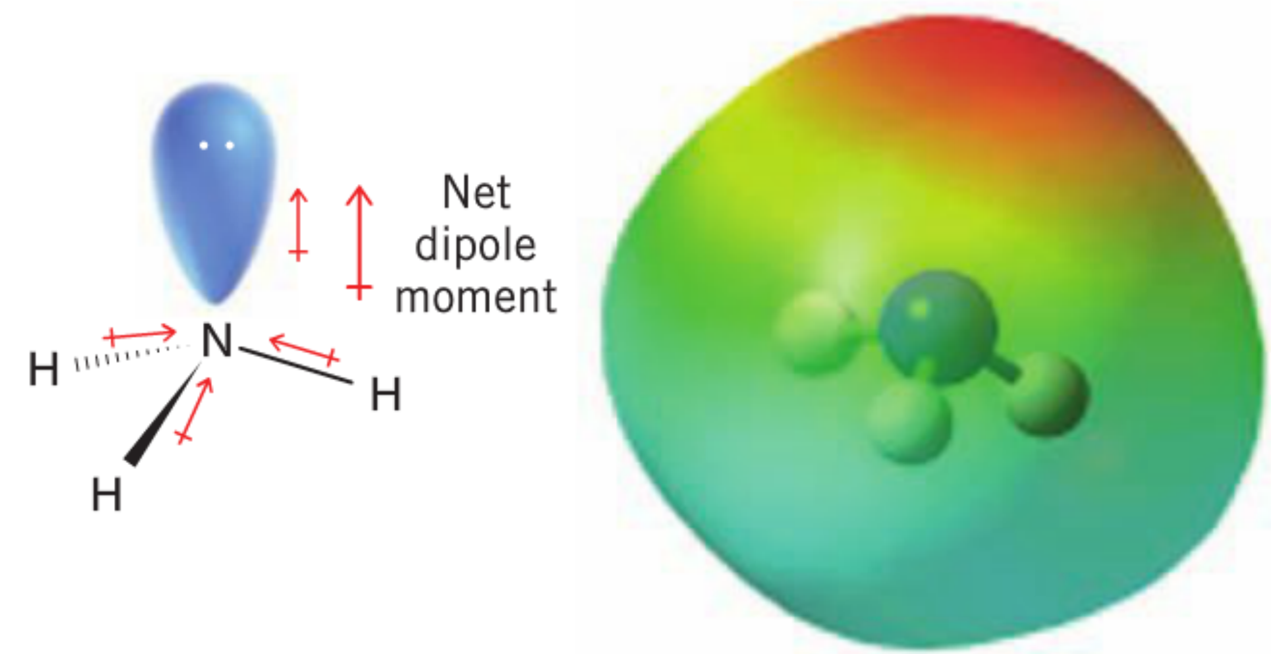
(a) (b)

Dipole Moments are Vectors

- Lone pairs create a dipole as seen in water and ammonia
- For water, the vector addition places the net dipole between the one pairs
- For ammonia, the dipole is in line with the lone pair
- What has a bigger dipole magnitude, NH3 or NF3???



Water



Ammonia

Dipole Moments

- The polarization in a bond or molecule is measure by a dipole moment
- A dipole moment is a measure of charge by distance
- A Debye (mu) is the unit of measure

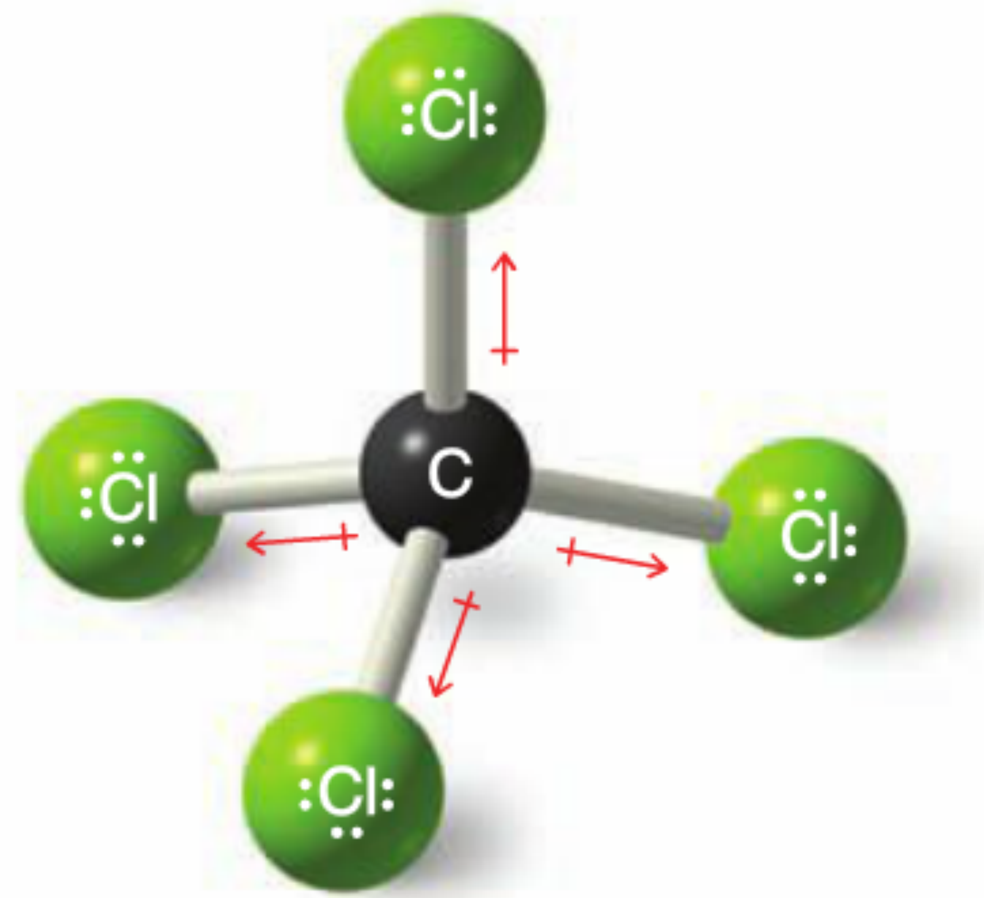
TABLE 2.1 DIPOLE MOMENTS OF SOME SIMPLE MOLECUL[illegible]

Formula	μ (D)	[illegible]	[illegible]
H_2	0	[illegible]	0
Cl_2	0	[illegible]	1.87
HF	1.83	[illegible]	1.55
HCl	1.08	$CHCl_3$	1.02
HBr	0.80	CCl_4	0
HI	0.42	NH_3	1.47
BF_3	0	NF_3	0.24
CO_2	0	H_2O	1.85

Why are some of these values 0?
Aren't there polar bonds here?

Non-Polar Molecules Containing Polar Bonds

- Carbon tetrachloride contains 4 polar covalent C-Cl bonds
- The molecule, however, has no net dipole moment (mu=0)
- ~~Huh?~~ Think about a game of tug-a-war...
- The Cl atoms all pull with equal magnitude to the four corners of the tetrahedron
- The dipole of each bond...
- ... Is canceled out by the others
- Symmetrical molecules like this can be non-polar despite having polar bonds
- Let's look at CO2 and BF3



$\mu = 0$ D

Dipole Moment???

- Which molecule would you expect to have a dipole?