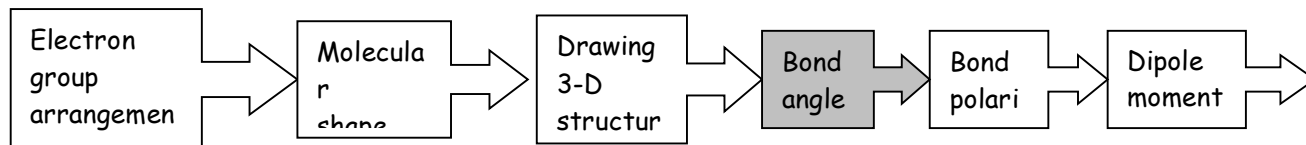


## WS 7 Valence Shell Electron Pair Repulsion (VSEPR): \_



A bond angle is the angle made by three connected nuclei in a molecule. By convention, the bond angle is considered to be between  $0^\circ$  and  $180^\circ$ . Electron domains have characteristic angles and structures. For example, a central atom with two regions of electron density is considered linear with a bond angle of  $180^\circ$ . Structures that are more complex have multiple angles. We start by examining the bond angles and regions of electron density of simple molecules. These orientations lead us to basic molecular shapes. Now we will examine the bond angles and regions of electron density of simple molecules and look for similarities that will lead to insight in molecular polarity.

### Part 1: Bond angles and electron domains

Table 1: Bond angles and bonding domains for some selected molecules

Molecular formula	Lewis structure	Bond angle	Bond angle value CACHe	# Regions of electron density	# Bonding domains	# Nonbonding domains
$\text{CO}_2$	$\text{O}=\text{C}=\text{O}$	$\angle\text{OCO}$	$180^\circ$	2	2	0
$\text{HCCH}$	$\text{H}-\text{C}\equiv\text{C}-\text{H}$	$\angle\text{HCC}$	$180^\circ$	2	2	0
$\text{ClNCl}$	$\text{Cl}-\text{N}=\text{N}-\text{Cl}$	$\angle\text{ClNN}$	$117.4^\circ$	3	2	1
$\text{NO}_3^-$	$\begin{array}{c} \text{O} \\   \\ \text{O}-\text{N}=\text{O} \end{array}$	$\angle\text{ONO}$	$120^\circ$	3	3	0
$\text{H}_2\text{CCH}_2$	$\begin{array}{c} \text{H} & & \text{H} \\ & \diagdown & / \\ & \text{C}=\text{C} \\ & / & \diagdown \\ \text{H} & & \text{H} \end{array}$	$\angle\text{HCH}$	$121.1^\circ$	3	3	0
$\text{CH}_4$	$\begin{array}{c} \text{H} \\   \\ \text{H}-\text{C}-\text{H} \\   \\ \text{H} \end{array}$	$\angle\text{CHC}$	$109.45^\circ$	4	4	0

Molecular formula	Lewis structure	Bond angle	Bond angle value CACHe	# Regions of electron density	# Bonding domains	# Nonbonding domains
CH <sub>3</sub> Cl		$\angle\text{HCCl}$ $\angle\text{HCH}$	109.45° 109.45°	4	4	0
CCl <sub>4</sub>		$\angle\text{ClCCl}$	109.45°	4	4	0
NH <sub>3</sub>		$\angle\text{HNNH}$	107°	4	3	1
PF <sub>3</sub>		$\angle\text{FPF}$	96.3°	4	3	1
H <sub>2</sub> O		$\angle\text{HOH}$	104.5°	4	2	2
SbF <sub>5</sub>		$a\angle\text{FSbF}$ $e\angle\text{FSbF}$	90° 120°	5	5	0
BrF <sub>5</sub>		$\angle\text{FBrF}$	84.8°	6	5	1
CF <sub>3</sub>		$\angle\text{FCIF}$	81.5	5	3	2

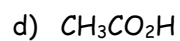
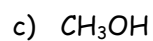
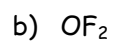
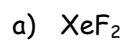
Bond angles calculated with MOPAC, CAChe. MOPAC calculations yield bond orders, bond lengths, and bond angles that are generally in good agreement with experimental evidence.

## Questions to get you thinking

1. How are the bonding domains on a given atom with a molecule determined?
2. The bond angles can be grouped, roughly around three values, what are these three values?
3. How is the number of non-bonding domains on a given atom with in a mole determined?
4. What correlation can be made between the values in the last two columns of the table above and the groupings from the last question?

5. Look at the information for ammonia and phosphorus tri-fluoride. They have the same molecular geometry. What is it? Are the bond angles the same? If they are not the same, explain why based on lone pairs and sizes of atoms. Nitrogen trifluoride has the same molecular geometry and a bond angle of  $102^\circ$ . Does this information fit into your theory about the differences in the bond angles?
6. Antimony penta-fluoride and bromine penta fluoride have the same number of fluorine's. Are their molecular geometries the same? How does this difference affect their bond angles?
7. Nitrate and nitrite have the same electron geometry but different molecular geometries. Thinking about electron pair repulsions, what can you conclude about bond angles based on these two molecules (polyatomic ions). You can draw a similar conclusion by examining the structures of ethane ( $C_2H_4$ ) and dinitrogen dichloride.  $\angle ClNCl = 117^\circ$  (close to  $120^\circ$ ) in  $ClN_2Cl$ .

8. Each of the following molecules has more than one "central atom". For each molecule, draw its Lewis structure. Determine the molecular shape and the electron pair geometry. When possible, give approximate bond angles.



## Part 4: Bond Polarity And Dipole Moments

Dipole moments of selected molecules

Molecule AB	Moment ( $\mu$ , D)	Geometry	Molecule AB <sub>2</sub>	Moment ( $\mu$ , D)	Geometry
HF	1.78	Linear	H <sub>2</sub> O	1.85	bent
HCl	1.07	Linear	H <sub>2</sub> S	0.95	Bent
HBr	0.79	Linear	SO <sub>2</sub>	1.62	Bent
HI	0.38	Linear	CO <sub>2</sub>	0	linear
H <sub>2</sub>	0	Linear			
		Linear			
Molecule AB <sub>3</sub>	Moment ( $\mu$ , D)	Geometry	Molecule AB <sub>4</sub>	Moment ( $\mu$ , D)	Geometry
NH <sub>3</sub>	1.47	Trigonal-pyramidal	CH <sub>4</sub>	0	Tetrahedral
NF <sub>3</sub>	0.23	Trigonal-pyramidal	CHCl <sub>3</sub>	1.04	Tetrahedral
BF <sub>3</sub>	0	Trigonal-planar	CH <sub>2</sub> Cl <sub>2</sub>	1.60	Tetrahedral
			CCl <sub>4</sub>	0	Tetrahedral
			CH <sub>3</sub> Cl	1.89	Tetrahedral
			CH <sub>3</sub> Br	1.82	Tetrahedral
			CH <sub>3</sub> I	1.62	Tetrahedral

1. Ammonia and nitrogen tri-fluoride have the same geometry. Thinking about the different bonds in the two molecules, what is the affect of the lone pair and these polar bonds on the overall dipole moment of the two molecules.
2. Looking at the dipole moment for boron tri-fluoride and nitrogen tri-fluoride, the number of atoms is the same, yet the dipole is very different. Explain why.
3. Explain the trend of the dipole moment for the molecules H—X.

4. Looking at the methane series for  $AB_4$ , what molecule has the largest dipole moment? Which one has the smallest, non-zero dipole moment? What is different about their structures? What is the effect of the differences on the dipole? Do you think the  $\angle HCCl$  and  $\angle HCH$  bonds are the same for all of the molecules? What about the  $\angle ClCCl$  bonds?
5. Based on the bond polarities for the methane series of  $CH_3X$ , predict the dipole moment of  $CH_3F$ .