

VSEPR and POLARITY

Lecture 6



Dr Ewa Kazimierska

e.kazimierska@uwtsd.ac.uk

VSEPR MODEL

Valence Shell Electron Pair Repulsion VSEPR

- used to predict the 3-D shape of a molecule from the orientation of electron pairs around central atom (those with more than one bonded atom)
- electron pairs orient themselves in a way to minimizes the repulsion and maximizes the distance between them
- to form a bond atoms must be near each other
- electrons form bonding and non-bonding groups around atoms

single bond

one pair

one group

double bond

two pair

one group

triple bond

three pairs

one group

lone pair

one pair

one group

Shape of a molecule determined by electron group repulsion around central atoms



PREDICTING SHAPES OF MOLECULES

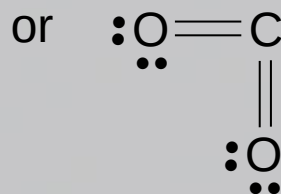
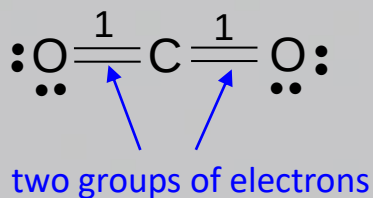
The following steps must be followed in order to decide the shape of a molecule

- put the **least electronegative atom** as a **central atom**
- count the **total number of electrons** in the outermost shell of the **central atom**
- count the **total number of electrons** in **other atoms** used to form bonds with the central atom
- **add** these two values to obtain the number of **valence shell electrons**
subtract an electron if the central atom has a **positive charge**;
add an electron for a central atom with a **negative charge**
- **halve** the count to get the **total electron pairs**

bond pair – bond pair < lone pair – bond pair < lone pair – lone pair



LEWIS STRUCTURES TO SHAPE

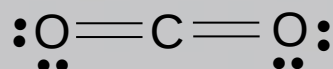
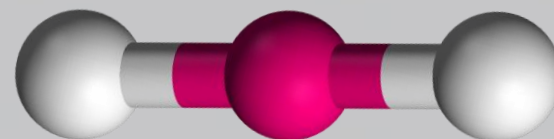


both fine Lewis structures

C – central atom (O more electronegative)

2 groups of electrons

The best way for them to get as far apart as possible



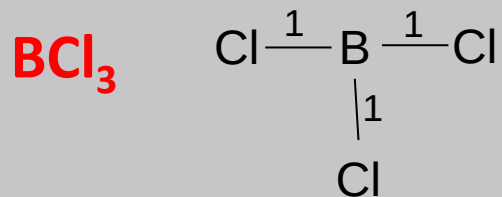
Electron Groups	Geometry	Shape	Angle (°)
2	Linear	—	180



VSEPR CHART

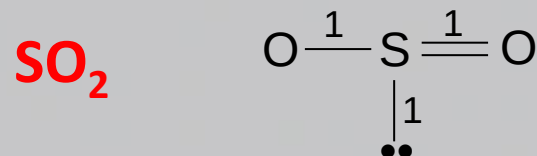
Electron Groups	Geometry	Bond/LP	Shape	Angle (°)
2	Linear	—— 2/0 ——	Linear	180





B - central atom

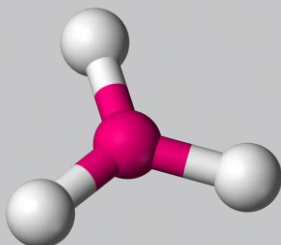
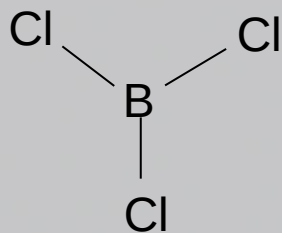
3 groups of electrons



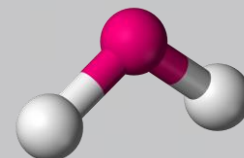
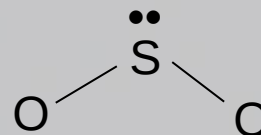
S - central atom

3 groups of electrons

The best way for them to get as far apart as possible



trigonal planar

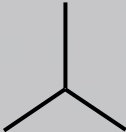


bent

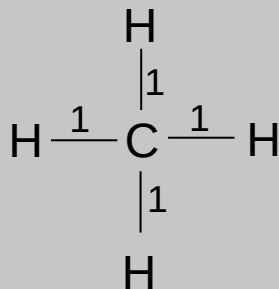
Electron Groups	Geometry	Shape	Angle (°)
3	trigonal planar		120
	bent (angular)		<120



VSEPR CHART

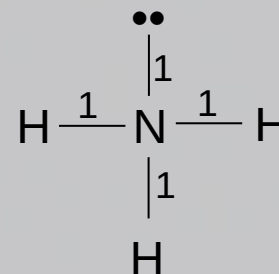
Electron Groups	Geometry		Bond/LP		Shape	Angle (°)
2	Linear		2/0		Linear	180
3	Trigonal planar		3/0		Trigonal planar	120
			2/1		bent (angular)	<120





C – central atom

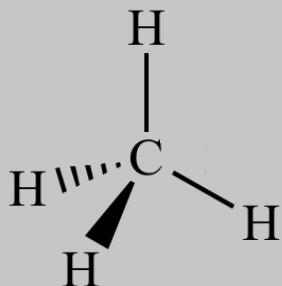
4 groups of electrons



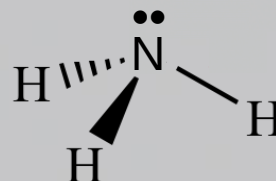
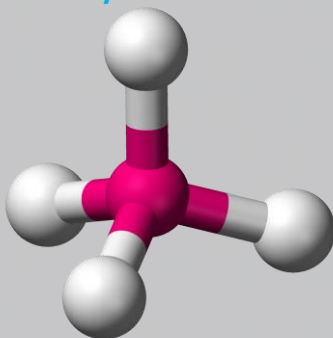
N – central atom

4 groups of electrons

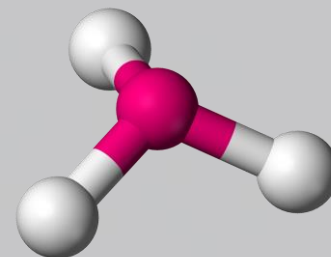
The best way for them to get as far apart as possible



tetrahedral



trigonal pyramidal



Electron
Groups

4

Geometry

tetrahedral

**trigonal
pyramidal**

Shape

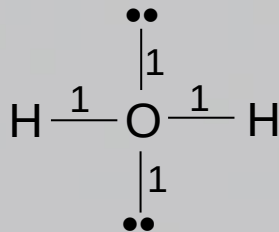
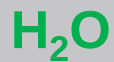


Angle (°)

109.5

<109.5





O – central atom

4 groups of electrons

Electron
Groups

4

Geometry

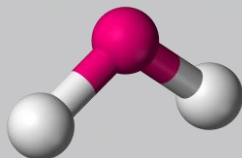
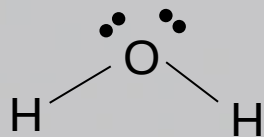
bent

Shape



Angle (°)

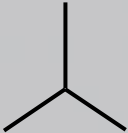
<109.5



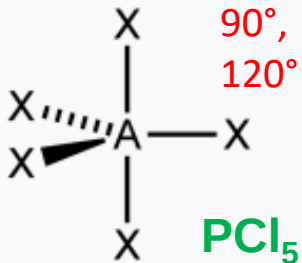
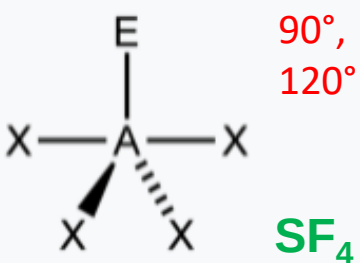
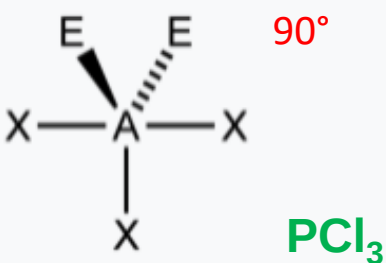
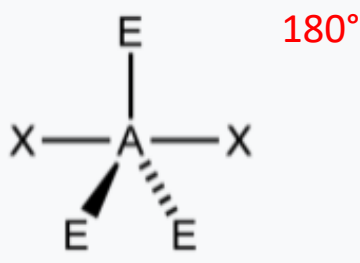
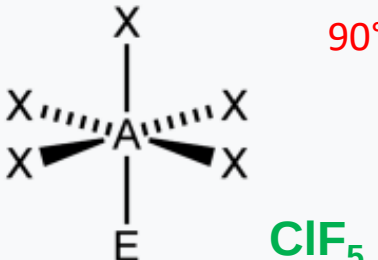
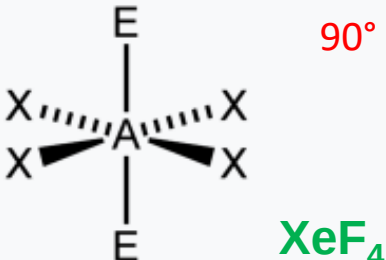
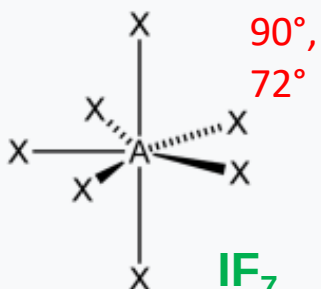
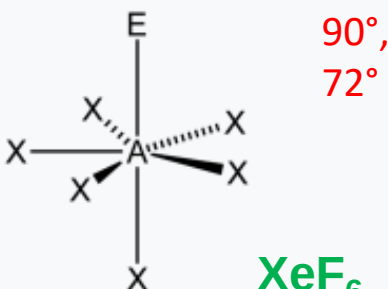
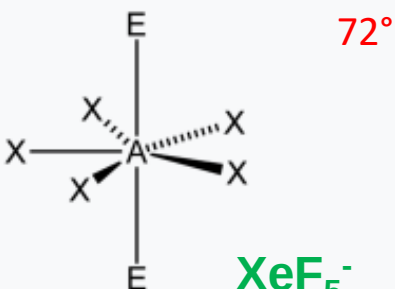
bent



VSEPR CHART

Electron Groups	Geometry		Bond/LP		Shape	Angle (°)
2	linear		2/0		linear	180
3	trigonal planar		3/0		trigonal planar	120
			2/1		bent (angular)	<120
4	tetrahedral		4/0		tetrahedral	109.5
			3/1		trigonal pyramidal	<109.5
			2/2		bent (angular)	<109.5



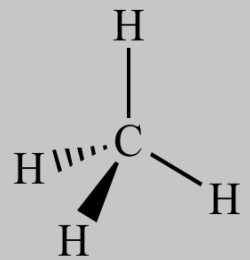
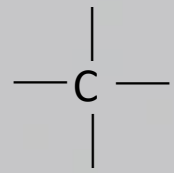
Steric number	Molecular geometry ^[13] 0 lone pairs	Molecular geometry ^{[1]: 413–414} 1 lone pair	Molecular geometry ^{[1]: 413–414} 2 lone pairs	Molecular geometry ^{[1]: 413–414} 3 lone pairs
5	 PCl₅ Trigonal bipyramidal	 SF₄ Seesaw	 PCl₃ T-shaped	 Linear
6	 SF₆ Octahedral	 ClF₅ Square pyramidal	 XeF₄ Square planar	
7	 IF₇ Pentagonal bipyramidal	 XeF₆ Pentagonal pyramidal	 XeF₅⁻ Pentagonal planar	



CARBON MOLECULES

Alkanes

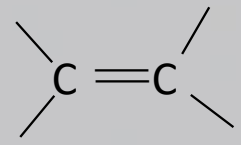
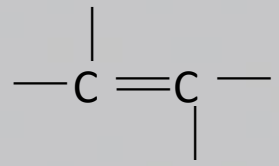
methane



TETRAHEDRAL

Alkenes

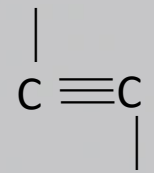
ethene
(ethylene)



TRIGONAL PLANAR

Alkynes

acetylene



LINEAR



POLAR MOLECULES

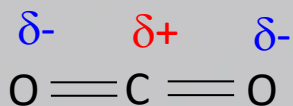
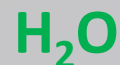
Bonds can be polar – one end $\delta+$ and the other $\delta-$ —————→ electronegativity differences

Molecules can be polar – one end $\delta+$ and the other $\delta-$ —————→ sum of polar bonds

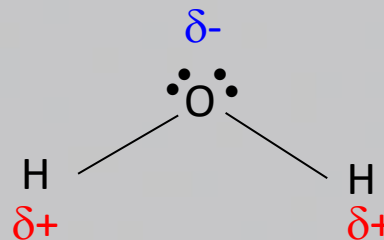
Polar molecules occur when two atoms do not share electrons equally in a covalent bond



vs



non-polar

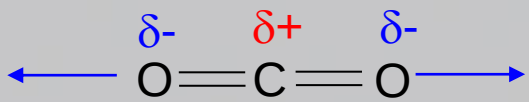


polar
has a dipole



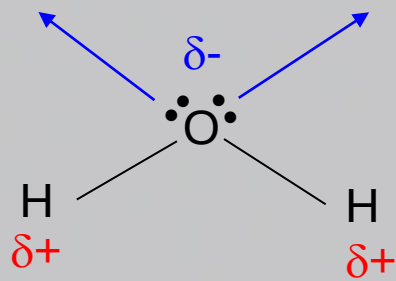
POLAR MOLECULES: Vectors

Polar bonds are treated as **vectors** (both direction and magnitude) pointing from the positively charged atom to the negatively charged atom.



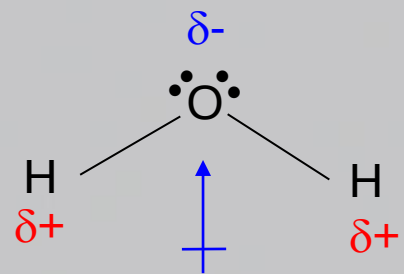
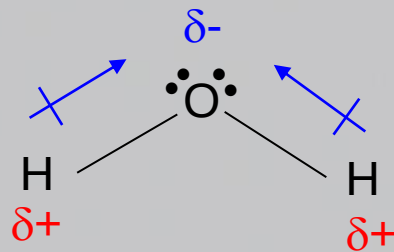
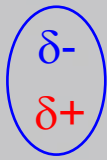
symmetrical distribution of polar bonds

cancel out
no dipole



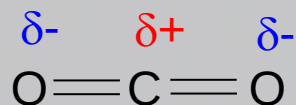
asymmetrical distribution of polar bonds

horizontal will cancel
vertical will not:



POLAR MOLECULES: Centre of charge

Polar covalent compounds have **two centres** of charges due to unequal sharing of electron pair.

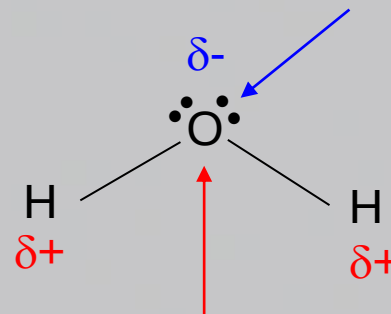


centre of δ^+ is the **carbon atom**

centre of δ^- is in the middle of O's
carbon atom

centres are same

no dipole



centre of δ^+ is in the middle of the H's

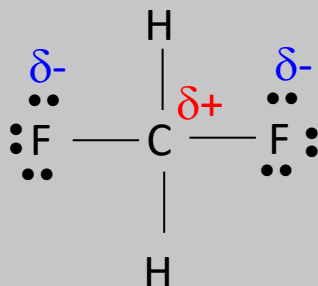
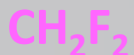
centre of δ^- is O atom

centres are different

dipole

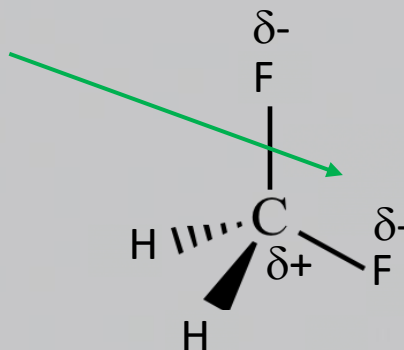
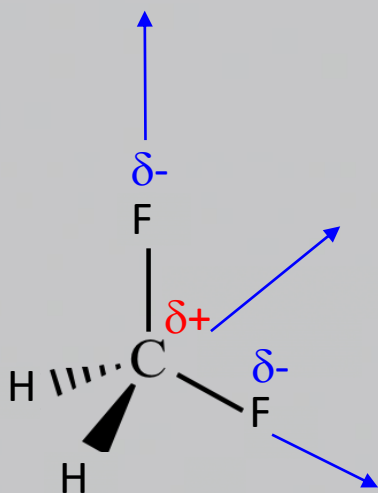


TOUGHER EXAMPLE



Non-polar?

tetrahedral geometry, which indicates the symmetric charge distribution around the central atom, the carbon atom.



Centre of $\delta+$ is the C atom
Centre of $\delta-$ is between F's

Centres are different

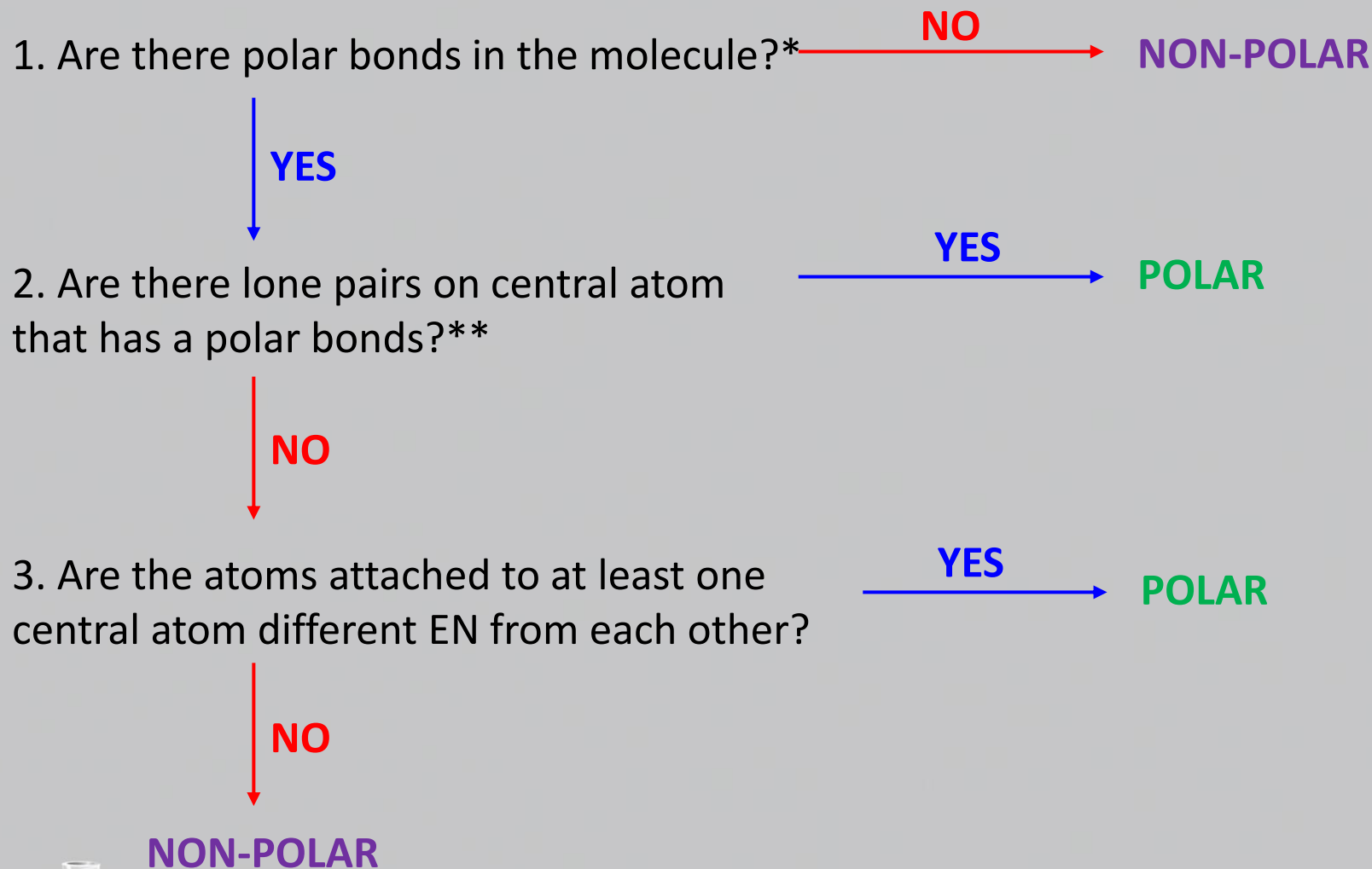
Dipole

POLAR !!!



The weak dipole of the C-H bond cannot cancel the effect of the strong dipole of the C-F bond. Hence, the difluoromethane molecule will have a net dipole moment despite its symmetrical tetrahedral geometry.

QUICK METHOD TO DETERMINE POLARITY

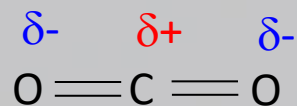


**Hydrocarbons non-polar*

***If lone pairs cancel out (linear, square planar, count this as no)*

1. Are there polar bonds in the molecule?

1. CO_2



Question 1.

Yes

Question 2.

No

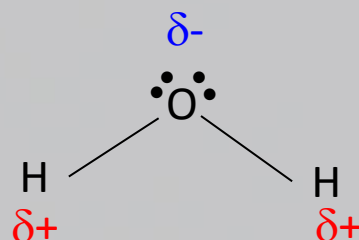
Question 3.

No

NON-POLAR

2. Are there lone pairs on the central atom that has polar bonds?

2. H_2O



Question 1.

Yes

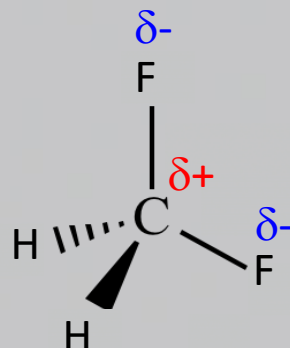
Question 2.

Yes

POLAR

3. Are the atoms attached to at least one central atom different EN from each other?

3. CH_2F_2



Question 1.

Yes

Question 2.

No

Question 3.

Yes

POLAR



Practice Problem 1: Using Lewis structures and VSEPR model, predict the shape of each of the following molecules:

- a) H_2S
- b) CS_2
- c) CF_3Cl
- d) GaI_3



Practice problem 2: Write the Lewis Structure and predict whether the molecule is polar or non-polar:

- a) CCl_4
- b) PF_3
- c) SO_2

