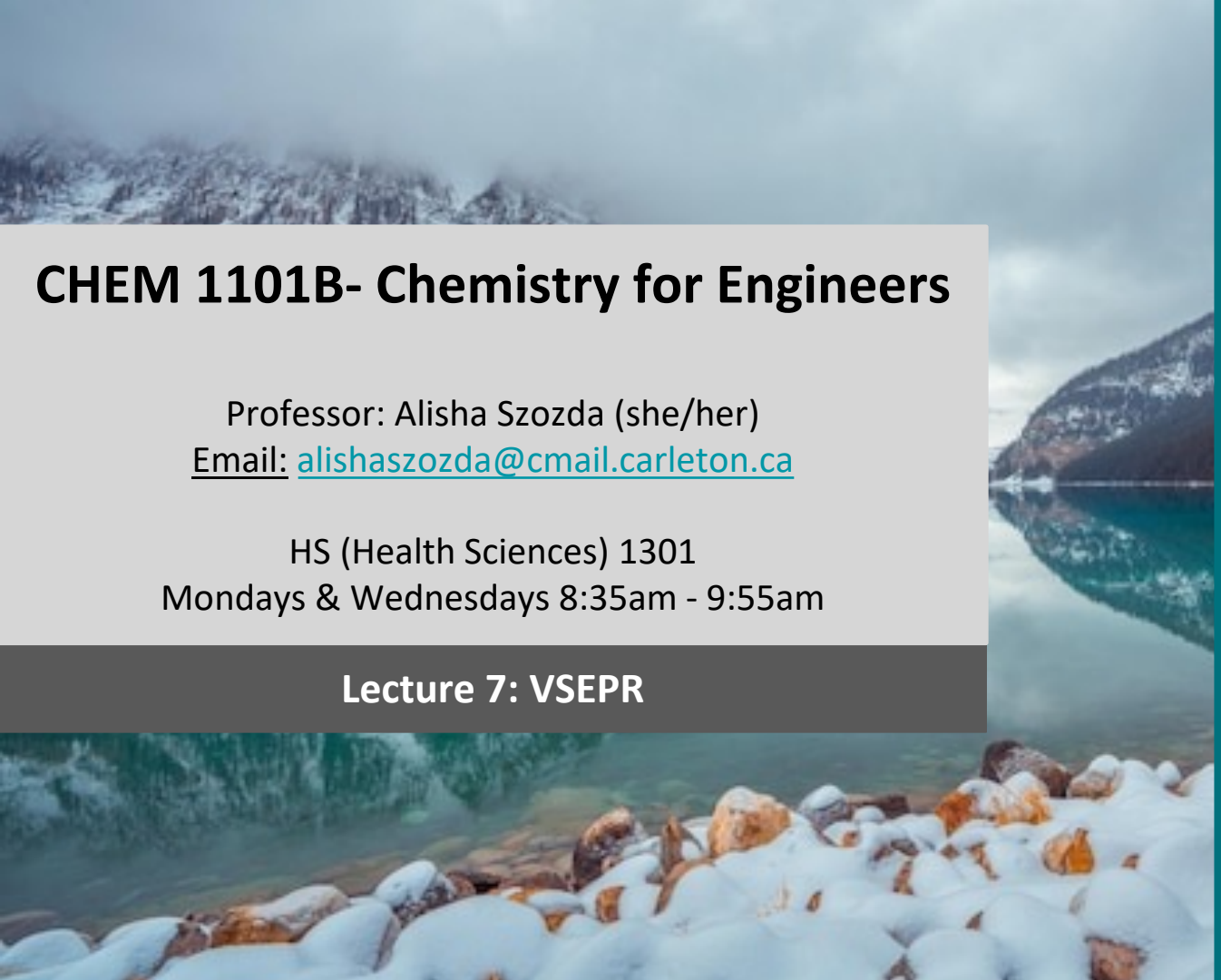


CHEM 1101B- Chemistry for Engineers

Professor: Alisha Szozda (she/her)
Email: alishaszozda@cmail.carleton.ca

HS (Health Sciences) 1301
Mondays & Wednesdays 8:35am - 9:55am

Lecture 7: VSEPR

Please feel free to introduce yourself to your neighbors– name, pronouns, a hobby, etc.

and/or

Answer the first question on Wooclap!

Learning outcome for Topic 7: The Molecule – VSEPR

LOs: (1) Use the VSEPR model to predict the shapes of molecules with steric #'s 2, 3, 4, 5, and 6.
(2) Predict bond and net dipoles

Last lecture…

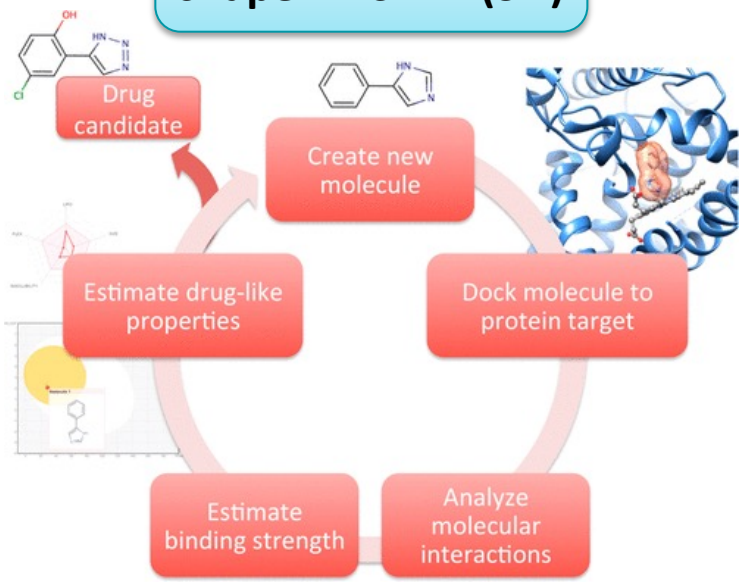
Lewis structures (2D)

Today's lecture…

Predicting the shape – VSEPR (3D)

Why is it important to understand 3D molecular structure?

- Shape affects how it interacts with other molecules
- Predict biological activity – to design drugs and decipher the function of the molecule



J. Chem. Educ. 2017, 94, 3, 335−344

VSEPR Theory – 3D Shapes of Molecules

VSEPR = Valence Shell Electron-Pair Repulsion

- Provides a way to predict the shape of molecules in 3D
- Each group of valence electrons around a central atom is located as far as possible from the others, to minimize repulsions.
- An electron pair or group = electrons that occupy a localized region in a molecule
- A ligand or outer atom = an atom (or group of atoms bonded to an inner atom)
- Steric number or number of electron pairs

  = the sum of the number of ligands plus number of lone pairs
  = total # of electron groups associated with atom

Drawing lewis structures to determine the steric number

To determine the steric number of a molecule, it is necessary to draw the Lewis structure. For example:

CH_3Cl H_2O

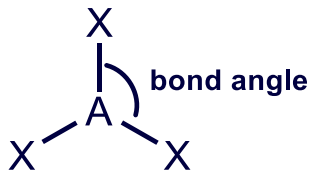
wooclap

What is the steric number for ClF_3?

The Molecular Shape

Once the steric number is known, we can determine the molecular shape.

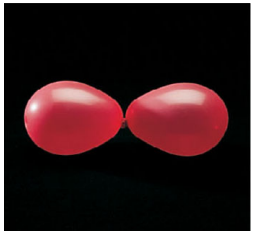
- Find the arrangement that maximizes the separation of electron groups from each other to minimize electron pair repulsions
- Defined by bond angles:



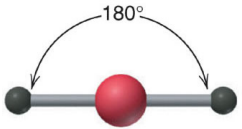
For example:

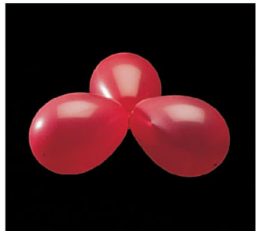
CH_3Cl H_2O ClF_3

5 Basic Electron Pair Geometries

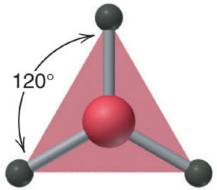


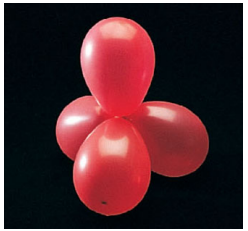
linear



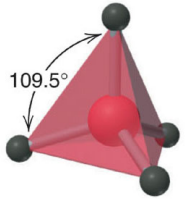


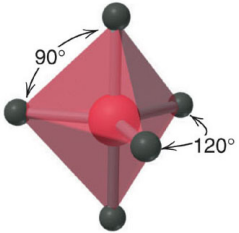
trigonal planar



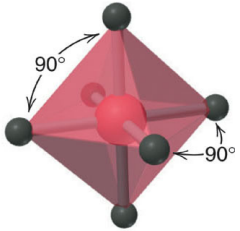


tetrahedral





trigonal bipyramidal

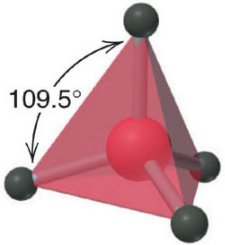


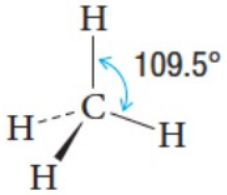
octahedral

Variations of the main geometries

Methane has a tetrahedral molecule shape (steric # = 4)

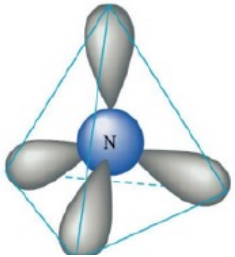
How does this compare to other molecules with same steric #?

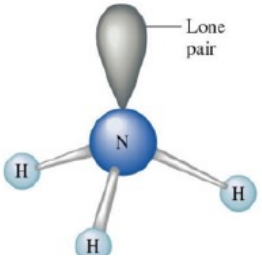


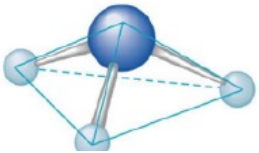


Example 1: Ammonia

- Unlike methane, one of ammonia's electron pairs is a lone pair

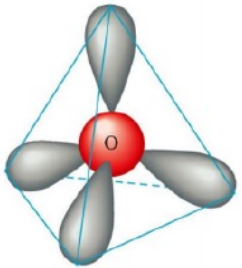


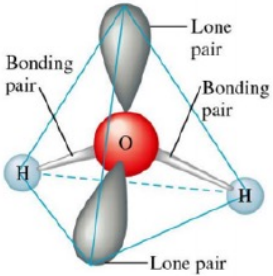


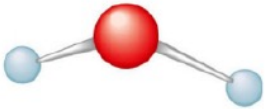


Example 2: Water

- Unlike methane, two of water's electron pairs are lone pairs







This affects the overall VSEPR shape

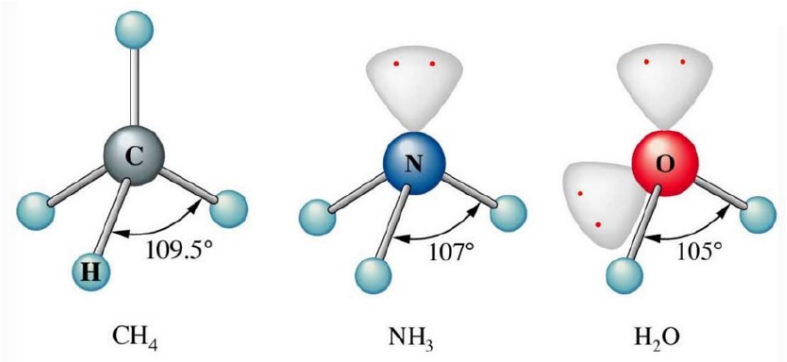
Bond angles are not always ideal

Electron pair geometries can differ from ideality, giving rise to differences in bond angles from those predicted from the ideal shapes.

- Electron groups with higher electron density will repel other groups more
- This pushes them further away from other groups
- This causes lower electron density groups to be closer to each other

In terms of decreasing repulsion: (LP = lone pair, BP = bonding pair)

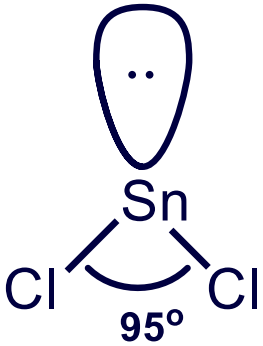
LP----LP > LP----BP > BP----BP

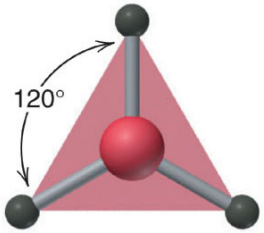


Other examples of non-ideal bond angles

For example:

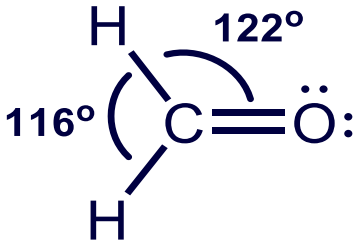
Non-bonding lone pairs



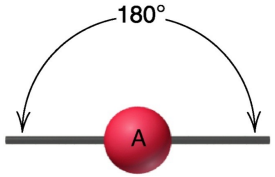
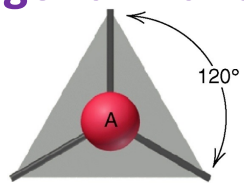
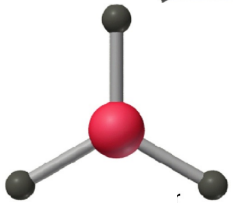
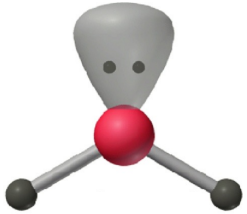


Trigonal Planar geometry

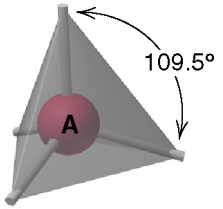
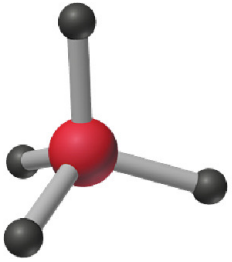
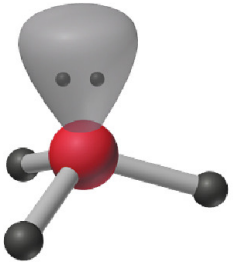
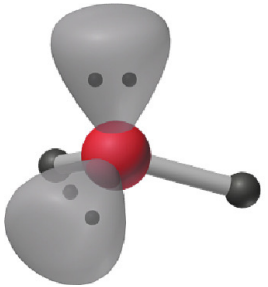
Double bonds



Shapes of Molecules: Steric Number = 2 or 3

	Linear	Trigonal Planar	
Electron pair geometry			
Molecular Shape			
	Linear	**Trigonal Planar**	**Bent**
Number of ligands	**2**	**3**	**2**
Bond Angle	**180°**	**120°**	**<120°**
Examples	**HCN** **BeF_2**	**SO_3** **CO_3^{2-}**	**O_3** **SO_2**

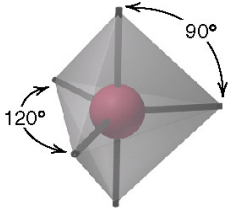
Shapes of Molecules: Steric Number = 4

Electron pair geometry	**Tetrahedral** 		
Molecular Shape			
	Tetrahedral	**Trigonal Pyramidal**	**Bent (V-shaped**
Number of ligands	**4**	**3**	**2**
Bond Angle	**109.5°**	**<109.5°**	**<109.5°**
Examples	**CH_4** **SO_4^{2-}**	**NH_3** **H_3O^+**	**H_2O** **SCl_2**

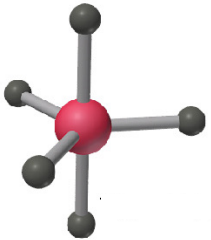
Shapes of Molecules: Steric Number = 5

Electron pair geometry

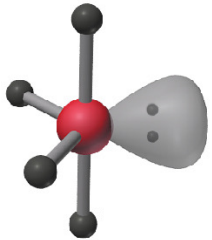
Trigonal Bipyramidal



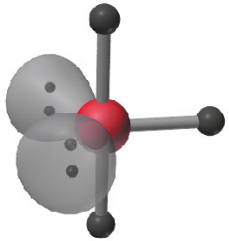
Molecular Shape



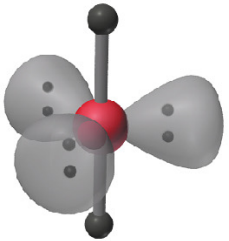
Trigonal Bipyramidal



Seesaw



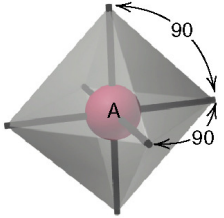
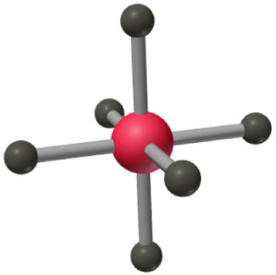
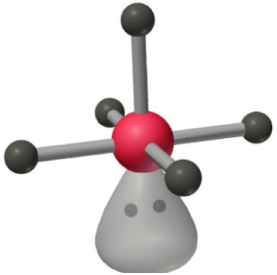
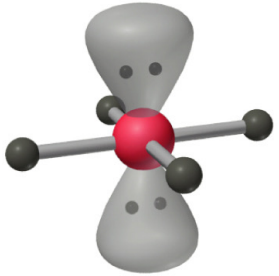
T-shaped

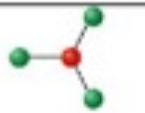
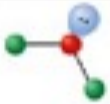
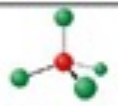
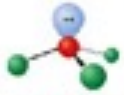
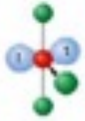
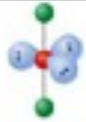
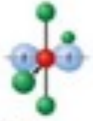
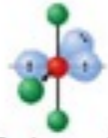
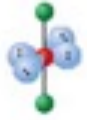


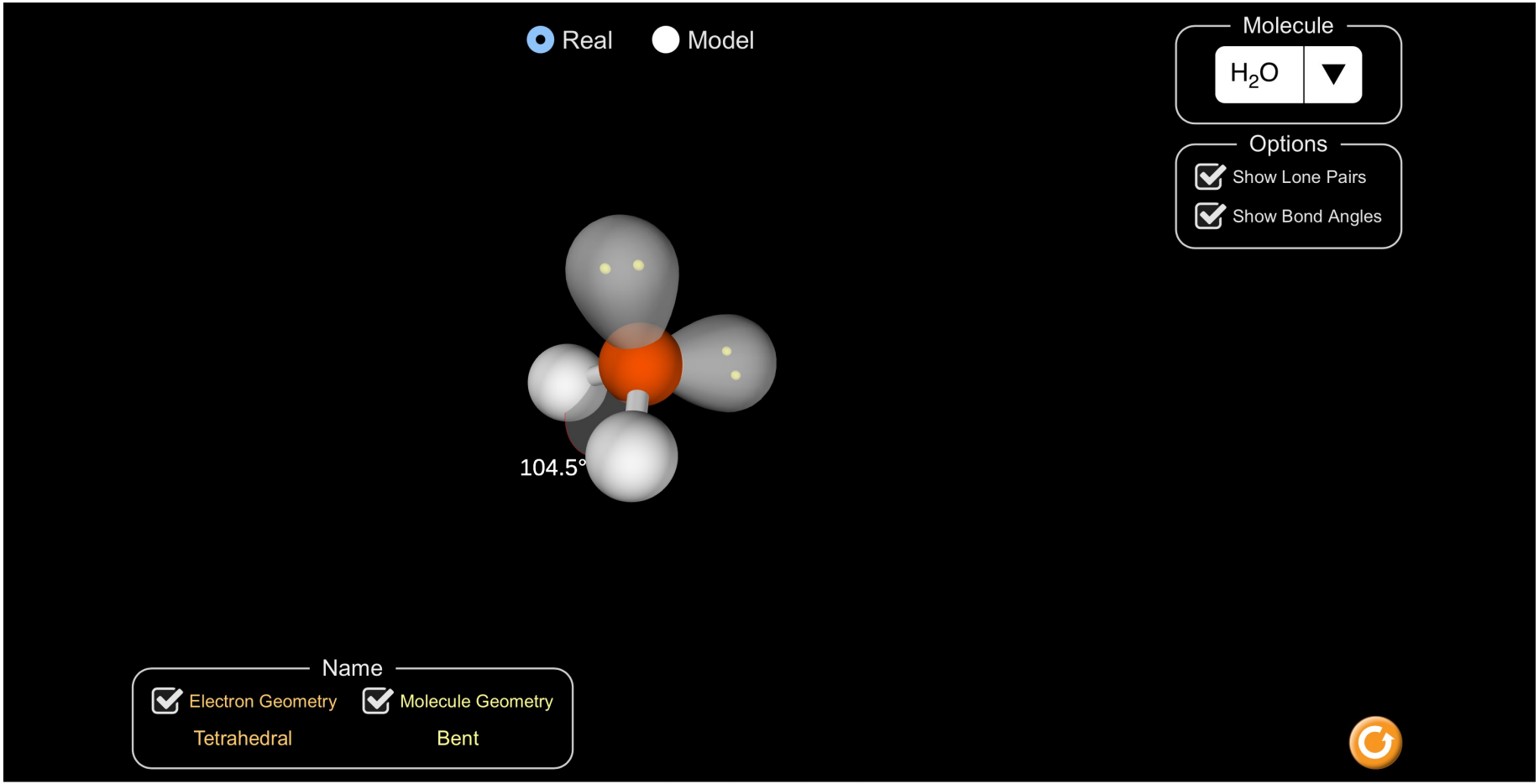
Linear

Number of ligands	**4**	**3**	**2**	**2**
Bond Angle	**120°** **90°**	**<120°** **<90°**	**<90°**	**180°**
Examples	**PF_5** **SOF_4**	**SF_4** **$IO_2F_2^-$**	**ClF_3** **BrF_3**	**I_3^-** **XeF_2**

Shapes of Molecules: Steric Number = 6

Electron pair geometry	**Octahedral** 		
Molecular Shape			
	Octahedral	**Square pyramidal**	**Square planar**
Number of ligands	**6**	**5**	**4**
Bond Angle	**90°**	**<90°**	**90°**
Examples	**SF_6** **IOF_5**	**BrF_5** **$XeOF_4$**	**XeF_4** **ICl_4^-**

Number of Electron Dense Areas	Electron-Pair Geometry	Molecular Geometry				
		No Lone Pairs	1 lone Pair	2 lone Pairs	3 lone Pairs	4 lone Pairs
2 	Linear	 Linear				
3 	Trigonal planar	 Trigonal planar	 Bent			
4 	Tetrahedral	 Tetrahedral	 Trigonal pyramidal	 Bent		
5 	Trigonal bipyramidal	 Trigonal bipyramidal	 Sawhorse	 T-shaped	 Linear	
6 	Octahedral	 Octahedral	 Square pyramidal	 Square planar	 T-shaped	 Linear



Molecule Shapes

Model

Real Molecules

https://phet.colorado.edu/sims/html/molecule-shapes/latest/molecule-shapes_en.html

VSEPR Terminology

wooclap

Electron pair geometry **Molecular Shape** **Electron group**

Steric Number **Ligand**

The electron group geometry of a compound is always governed by:

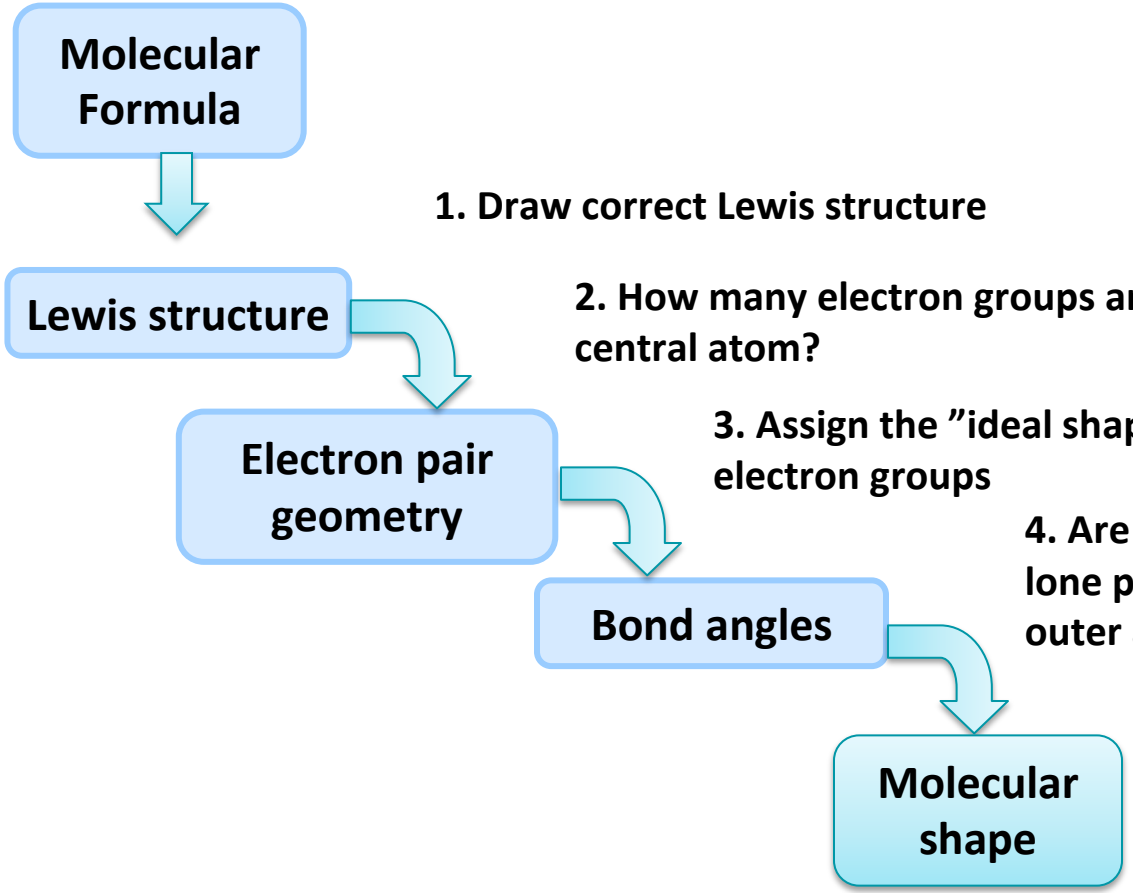
a) the number of electron groups.

b) the number of ligands.

c) the molecular shape.

d) the steric number.

Steps for applying the VSEPR Theory



Practice: Drawing molecular shapes

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Draw the molecular shapes for:

CS_2 $PbCl_2$

What is the bond angle in SF_2?

a) 180^o
b) 120^o
c) 109.5^o
d) $<120^o$
e) $<109.5^o$

More Molecular Shape Examples

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Draw the molecular shape for:

C_3H_4

What is the molecular geometry of SF_4?

A) tetrahedral
B) trigonal bipyramidal
C) see-saw
D) T-shape
E) linear

Putting it all together: Geometry for polyatomic molecules

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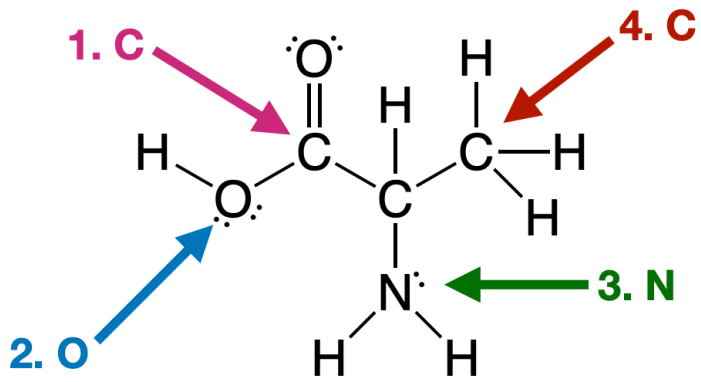
Alanine, an amino acid:



What is the molecular geometry of 4.C indicated with a red arrow?

A) Trigonal planar
B) Bent
C) Square planar
D) Trigonal pyramidal
E) Tetrahedral

Molecular Polarity

To predict whether a specific molecule is polar or non-polar you must consider two characteristics:

1) Type of bonds in the molecule (polar or non-polar)
2) Geometric shape of the molecule (VSEPR)

Bonds are polar if:

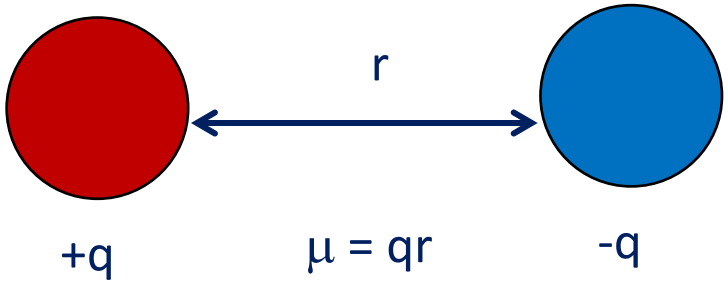
- Bonded atoms have different electronegativities
- More electronegative atoms have greater tendency to attract electrons (larger $\Delta\chi$)

Molecules are polar if:

- they contain one or more polar bonds
- the individual **bond dipoles** do not cancel (depends on the molecular shape), creating a **net dipole**

How polar is my molecule?

Dipole Moment, μ



Molecular shape + Δχ

↓

Polarity

(measured as the dipole moment, μ)

e.g. Cl_2

Δχ = 0

μ = 0 D

Non-polar

e.g. HCl

Δχ = 1.9

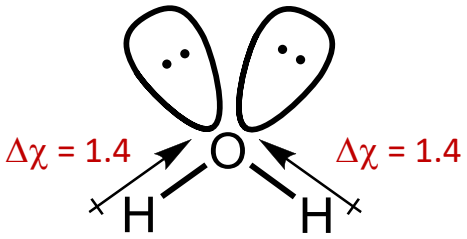
μ = 1.07 D

polar

- the larger the dipole moment (μ), the more polar the molecule
- units of polarity are debye (D)
  1 Debye = 3.34×10^{-30} C m

Polar versus nonpolar molecules

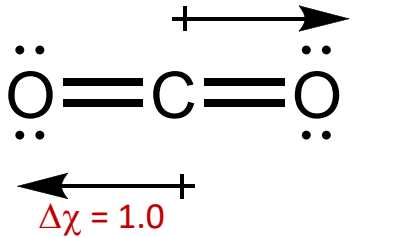
Water



- Water has a bent molecular structure and polar bonds between O --- H
- As a result, the dipoles add together to give the water molecule a net dipole

Molecules that have net dipoles are polar

Carbon Dioxide



- Carbon dioxide has a linear molecular structure and polar bonds between C --- O
- Since the polarities of these bond are equal and opposite, they cancel each other out

Molecules that have no net dipoles are non-polar

Which molecules are polar?

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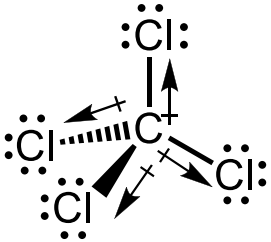
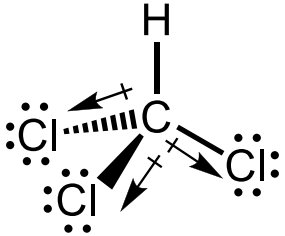
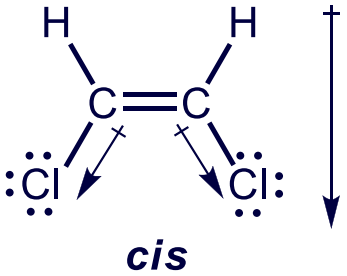
A.



B.

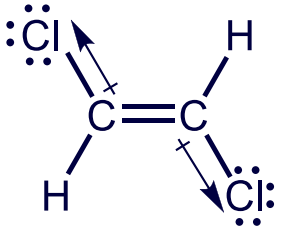


C.



cis

D.



trans

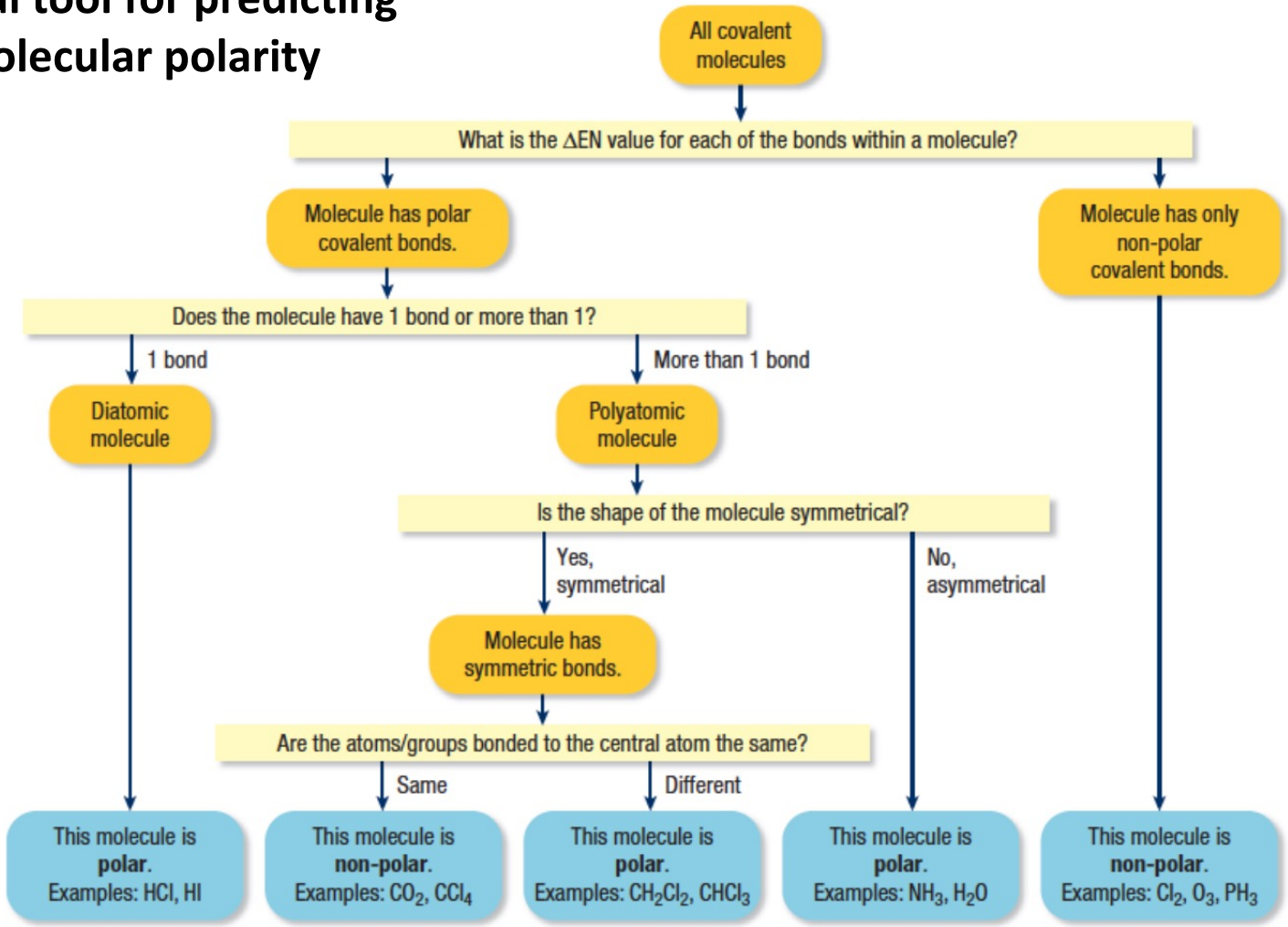
More examples: Which molecules are polar?

I_3^-

NO_3^-

Remember: Lone pairs DO NOT contribute to dipole moments by themselves.
NON-ZERO formal charges DO (in the direction of a negative and away from a positive F.C.)

Helpful tool for predicting molecular polarity



Using VSEPR Theory to detect explosives

Behind the Scenes at MIT; http://chemvideos.mit.edu

Detecting Explosives to Save Lives in War Zone

Stefanie explains how her research on designing sensors for explosives depends on the principles of VSEPR (valence shell electron pair repulsion) theory. Stefanie' s sensor design amplifies small-scale changes in bond angles following interaction with a target molecule, and she hopes that her work will lead to better detectors for landmines and improvised explosive devices.

https://youtu.be/L-2wcCFX77s?si=0vVQroJMDSY2Kc9k

https://chemvideos.mit.edu/real-world-applications/#colorbox