LECTURE 11. AN INTRODUCTION TO VB AND VSEPR THEORY

Now that we can draw 2-dimensional structures using Lewis dot structures, how do we make them into 3-dimensions?
Answer:

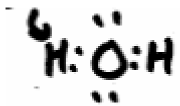
VSEPR (Valence Shell Electron Pair Repulsion) Theory

VSEPR says, around any central atom, electron rich regions tend to move as far from each other as possible.

What are electron rich regions?

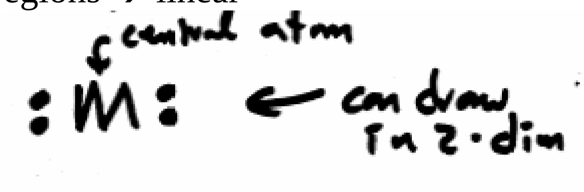
•• with a bond

•• with no bond →

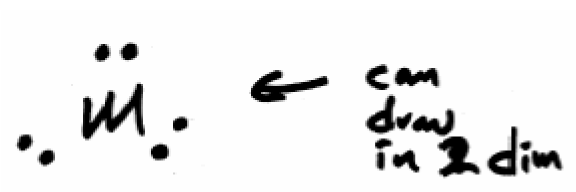


There are 5 examples of VSEPR to consider:

- 2 e- rich regions → linear

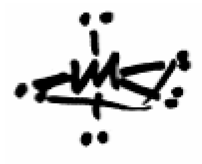


- 3 e- rich regions → trigonal planar

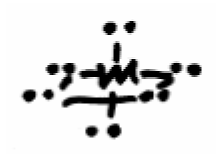


- 4 e- rich regions → tetrahedral

- 5 e- rich regions → trigonal bipyramidal



- 6 e- rich regions → octahedral



An exception to simple bond angles.

B and U e- pairs are not the same. If an e- pair is constrained by two nuclei, it takes less space than if constrained by one nucleus.

Bonding e- pair

Unbonded e- pair takes up more spac

So in H_2O, the •• takes up more space than the H**:**

Larger than

Smaller than 109.5

This compresses the O-H bonds to form a smaller H-O-H bond angle, about 105 degrees instead of 109.5 degrees. BUT, averaging of bond angles is still 109.5 degrees.

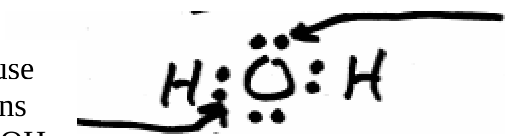
Now on to More Advanced VSEPR ideas as we ooze into Valence Bond (VB) Theory:

Molecular geometries	(pretty hard)
Multiple central atom	(pretty easy)
Hybrid orbits (VB theory)	(kind of hard)
Atomic orbits forming molecular orbits	(really hard)

Molecular Geometries

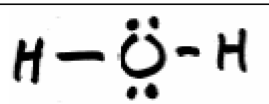
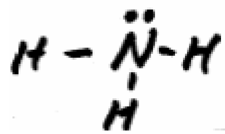
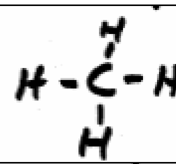
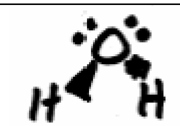
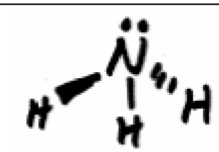
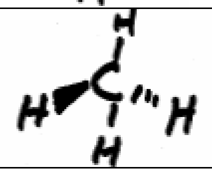
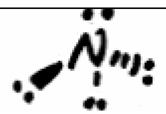
Looks at what happens when you distinguish **<u>B</u>**onding from **<u>U</u>**nbonded e- pairs.

B because electrons from an OH bond

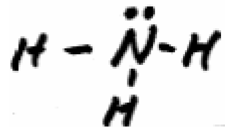
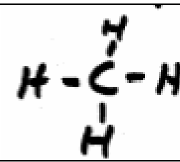
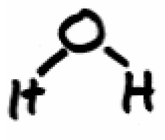
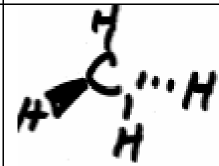
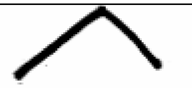
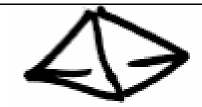
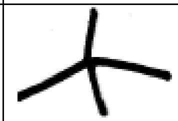


U because electrons from an unbonded pair on the O

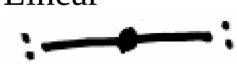
Consider three tetrahedral compounds (4 e- rich regions)

	H20	NH3	CH4
In 2-D			
In 3-D			
Electron rich regions	4	4	4
Electronic shape			
All are the same	Tetrahedral	Tetrahedral	Tetrahedral
Bond angle	109.5	109.5	109.5
Hybridization	sp3	sp3	sp3

So what is different? the number of B and U electrons.

			
# of B and U electrons	AB_2U_2	AB_3U	AB_4
So, draw without U, only B			
Notice the shape of the molecule			
Molecular geometry	Angular	Pyramidal	Tetrahedral

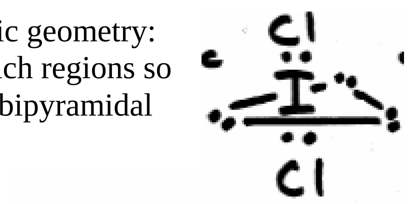
You can find all the different molecular shapes at the end of these notes. They have shapes that make sense.

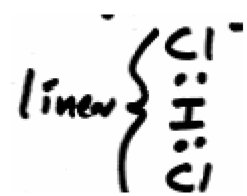
Linear  AB2	Trigonal 	Angular 	Tetrahedral 	T-shaped

AB2U3	AB3	AB2U AB2U2	AB4	 AB3U2
See-saw  AB4U	Trigonal Bipyramidal  AB5	Square planar  AB4U2	Square pyramidal  AB5U	Octahedral  AB6

Example: What is electronic and molecular geometry for ICl_2^-?
Note: ICl_2^- is like I_3^- and has 22 available electrons.

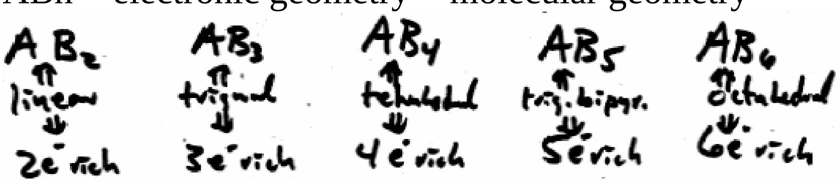
Electronic geometry:
note 5e- rich regions so
trigonal bipyramidal





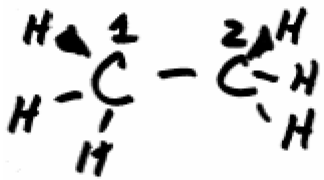
Molecular geometry:
of the form AB2U3,
ignore U3 → linear

Oh, and a hint to learn 5 types of molecular geometries when there are no unbonded pairs:
ABn = electronic geometry = molecular geometry

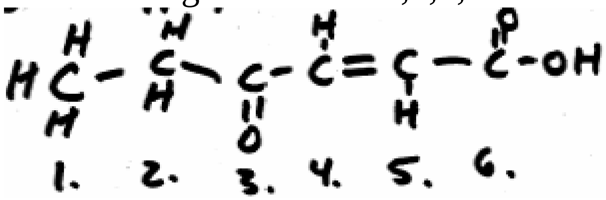


Multiple Central Atoms—this is a lot simpler than you might think

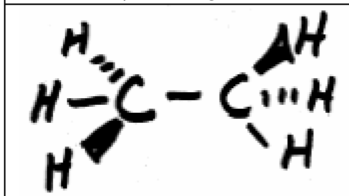
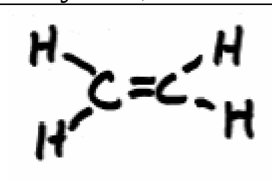
- just treat as individual central atoms looking only at neighboring e- rich regions.
  - Example: has 2 central atoms
  - Central atom 1 and 2 both have 4 e- rich regions, so they are both tetrahedral.



- can apply to large organic molecules
- tetrahedral atoms: 1, 2
- trigonal atoms: 3,4,5,6



The 3 famous multiple central atoms you must know COLD for this exam:

Ethane, C_2H_6	Ethylene, C_2H_4	Ethyne, C_2H_2
		
Tetrahedral	Trigonal planar	Linear
109.5	120	180
sp3	sp2	sp
All 7 sigma bonds	1 pi bond 5 sigma bonds	2 pi bonds 3 sigma bonds