Grades: 1 Exam, 3 Quizzes, 3 Labs, 4 Weeks Hwk

275 points (1245 in course)

EI, Ave=87, Range: 44-137

A	100
B	70
C	50
D	40

Q1	6.0
Q3	4.1

H_Exp 1	18.8
H_Exp 2	17.3
LM_3	17.9

Class Averages

EI	87	58%
QUIZ	10.2	51%
LAB	54.6	91%
HWK	34.3	76%

Course Grade Estimate

A	75%
B	65%
C	50%
D	40%

Bonding, Lewis Structures______________ Z Ch 12.15, 13

"There are therefore Agents in Nature able to make the Particles of Bodies stick together by very strong Attractions. And it is the Business of Experimental Philosophy to find them out." **Isaac Newton, 1717**

"Two atoms may conform to the rule of eight, or the octet rule, not only by the transfer of electrons from one atom to another, but also by sharing one or more pairs of electrons. These electrons which are held in common by two atoms may be considered to belong to the outer shells of both atoms." **Gilbert Newton Lewis, 1916**

"We shall say that there is a chemical bond between two atoms or groups of atoms in case that the forces acting between them are such as to lead to the formation of an aggregate with sufficient stability to make it convenient for the chemist to consider it as an independent molecular species." **Linus Carl Pauling, 1939**

(Nobel Prize in Chemistry in 1954 "for his research into the nature of the chemical bond and its application to the elucidation of the structure of complex substances" and Nobel Peace Prize in 1962.)

Seven SIMPLE BONDING CONCEPTS

13.11 – Resonance
13.12 – Exceptions to Octet Rule, FC
13.13 – VSEPR

lab reports
cover sheets
this week, next week

Seven SIMPLE BONDING CONCEPTS

1) **Lewis structures** – guidelines (13.10 – 13.12)

- determine total **number of valence electrons** from group numbers (GN); most atoms obey **octet rule** – exceptions to octet rule:

  2 – H, He
  4 – Be
  6 – B, Al
  species with odd number of electrons
  some species with an element beyond 2nd period

- draw structure with all bonding pairs and lone pairs using symmetry
- show all **resonance structures** (atoms do not move)
- determine **formal charge** (FC) on all atoms having any

  FC = GN – number of lone pair electrons – ½ number of bonding pair electrons

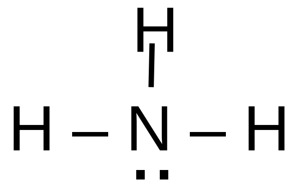
- **valence shell expand** (VSE) if atom is beyond 2nd period and 1) has a formal charge separation or 2) octet rule gives insufficient number of bonding electrons; VSE to minimize FC separation while maximizing number of resonance structures (VSE for Week 6)

this week

1) Lewis Structures

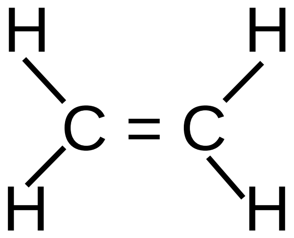
1. NH_3

VAL = 5 + 3 = 8 (/2 = **4** pairs)



2. C_2H_4

VAL = 2(4) + 4 = 12 (/2 = **6** pairs)

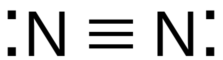


3. C_2H_2

VAL = 2(4) + 2 = 10 (/2 = **5** pairs)

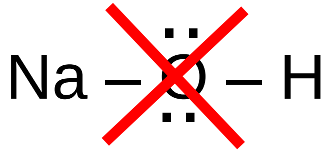
4. N_2

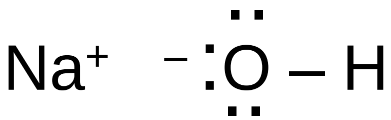
VAL = 2(5) = 10 (/2 = **5** pairs)



5. NaOH

VAL = 1 + 6 + 1 = 8 (/2 = **4** pairs)





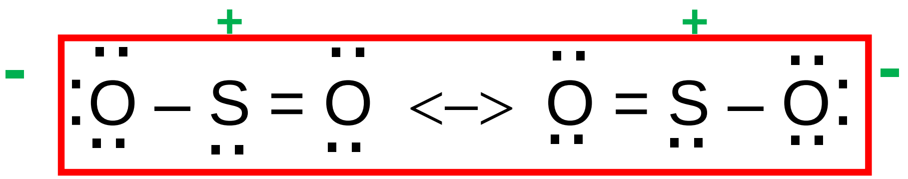
6. SO_2

VAL = 2(6) + 6 = 18

STAB = 3(8) = 24

BOND = 24 - 18 = 6 (/2 = 3 bp)

LONE = 18 - 6 = 12 (/2 = 6 lp)



RES

FC(S) = 6-2-6/2 = +1

FC(O) = 6-6-2/2 = -1

To Always Obtain the Optimal Octet Structure

1. VAL (total number of valence electrons) = sum of the valence electrons of each element (sum of the group numbers, GN) - charge (if an ion).
2. STAB (stable noble gas configuration) = sum of the electrons in the noble gas configuration for each element (2 for H, 8 for C and beyond). Since an atom achieves its greatest stability and lowest energy when it has a filled shell, the noble gas configuration, we assume that an atom in a molecule or ion will also be most stable when it has its noble gas complement of electrons around it - the ubiquitous "octet" rule.
3. BOND (total number of bonding electrons) = STAB - VAL and BP (number of bond pairs) = BOND/2. Since electrons are shared between atoms that are bonded together the "octet" around each atom over counts the actual number of electrons involved. The amount of over counting is the number of bonding electrons.
4. LONE (total number of lone pair electrons) = VAL - BOND and LP (number of lone pairs) = LONE/2. Valence electrons are of two varieties: they are either bonding electrons (BOND) or nonbonding, lone electrons (LONE).
5. Draw the Lewis structure using your calculated BP and LP. Remember that nature likes symmetry, put the odd atom in the center. The central atom will generally be the less electronegative (more electropositive) element.

2) Resonance, 3) Formal Charge

resonance – all resonance structures have same number of bonds and lone pairs

formal charge – usually more electronegative element has negative charge; consider CO

VSEPR Theory

Z Ch 13.13

"... the size of the valency group ... assume that the electron pairs occupy much the same positions whether they are shared or not ... determines, the type of spatial arrangement adopted ... With a quartet of electron , the molecule is linear (as in Cl-Hg-Cl). With a sex-tet, the arrangement is planar, and the valency angles 120°, giving with a covalency of 3 the plane symmetrical molecule (as in BF_3) and where it is 2-covalent, as in $SnCl_2$ a triangular mole-cule. With an octet there appear[s] ... the tetrahedron ..., the 2-covalent being triangular and the covalent pyramidal ... The decet when fully shared (5-covalent) gives the trigonal [bi]pyramid ... The 2-covalent decet is ... linear, as if derived from the trigonal bipyramid by removing all three equatorial groups. The duodecet when fully shared (6-coval-ent) is octahedral ... The 4-covalent form is ... square, and so to be derived from the octahedron by removing two trans groups."

Nevil V. Sidgwick and Herbert M. Powell, 1940

"The stereochemistry of an atom in any particular molecule depends on the number of pairs of electrons in its valency shell ... The gen-eral arrangement of the valencies around any atom is determined by the fact that the lone pairs ... arrange themselves as far apart as possible ... A more detailed and exact description of the shapes of molecules can be given if it is assumed ... that a lone pair repels other electron pairs more than a bonding pair of electrons ..."

Ronald J. Gillespie and Ronald S. Nyholm, 1957

"We were concerned about how to best give students some understanding of the shapes of inorganic molecules ... We found that we could explain the shapes of essentially all molecules of the type AX on the basis that the electron pairs in the valence shell of a central atom keep as far apart as possible. Moreover, by making allowances for the differences between bonding and nonbonding electron pairs, we could account for small deviations from the basic idealized shapes ..."

Ronald J. Gillespie, 1984

4) **V**alence **S**hell **E**lectron **P**air **R**epulsion (**VSEPR**) Theory

electrons repel one another

4) **V**alence **S**hell **E**lectron **P**air **R**epulsion (**VSEPR**) Theory

repulsions: BP/BP < BP/LP < LP/LP

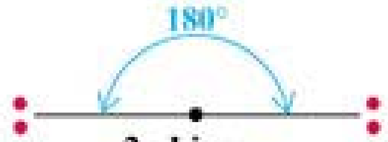
steric number (number of electron pairs) => **electronic geometry**

molecular geometry (shape) => bond angles, distortions

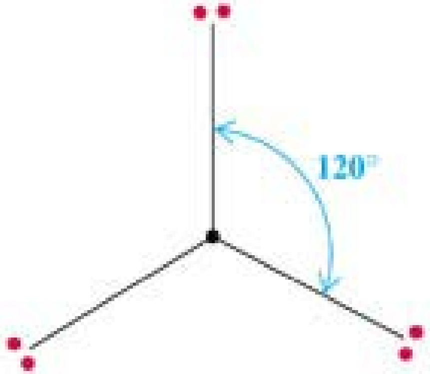
electronegativity => bond polarity

molecular polarity => dipole moment

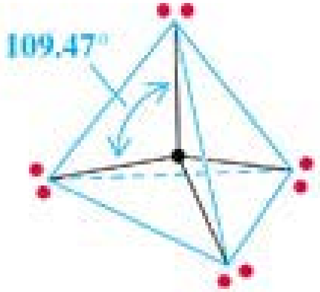
Electrons Repel One Another



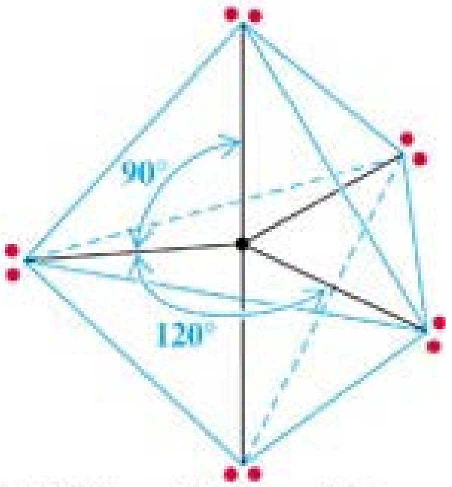
2: Linear



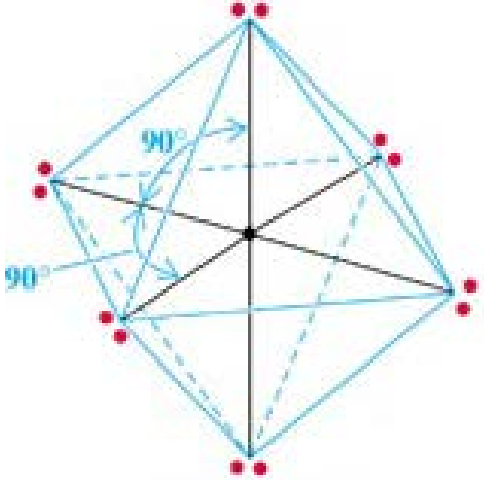
3: Trigonal planar



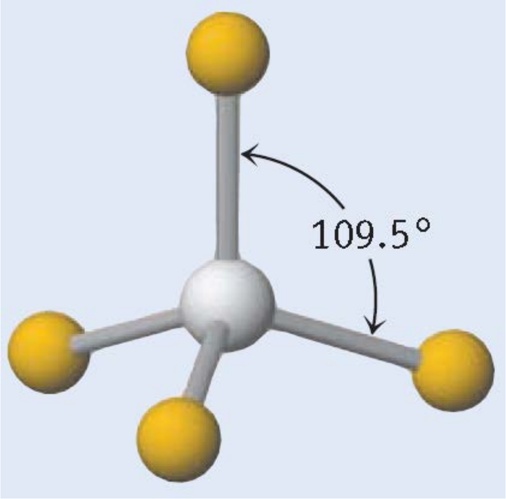
4: Tetrahedral



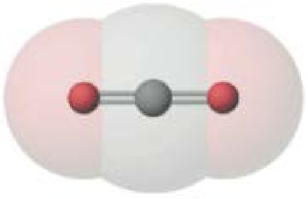
5: Trigonal bipyramidal



6: Octahedral

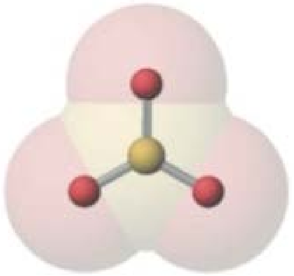


Electronic Geometry: Linear (SN=2)



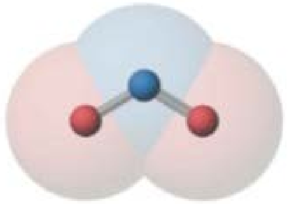
CO_2

Electronic Geometry: Trigonal Planar (SN=3)

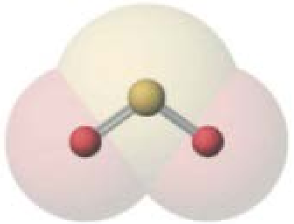


SO_3

Molecular Geometry: Bent (Angular)

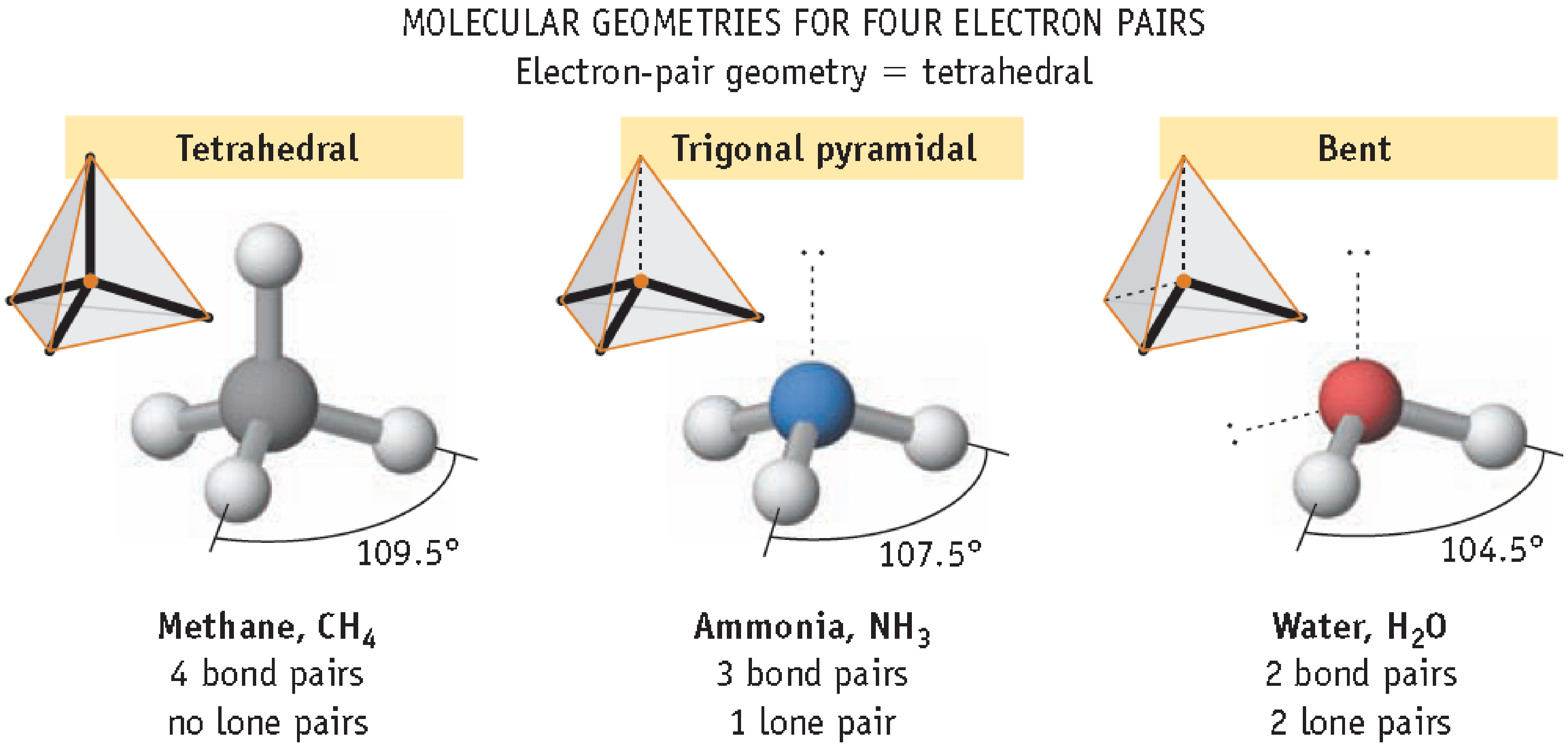


NO_2



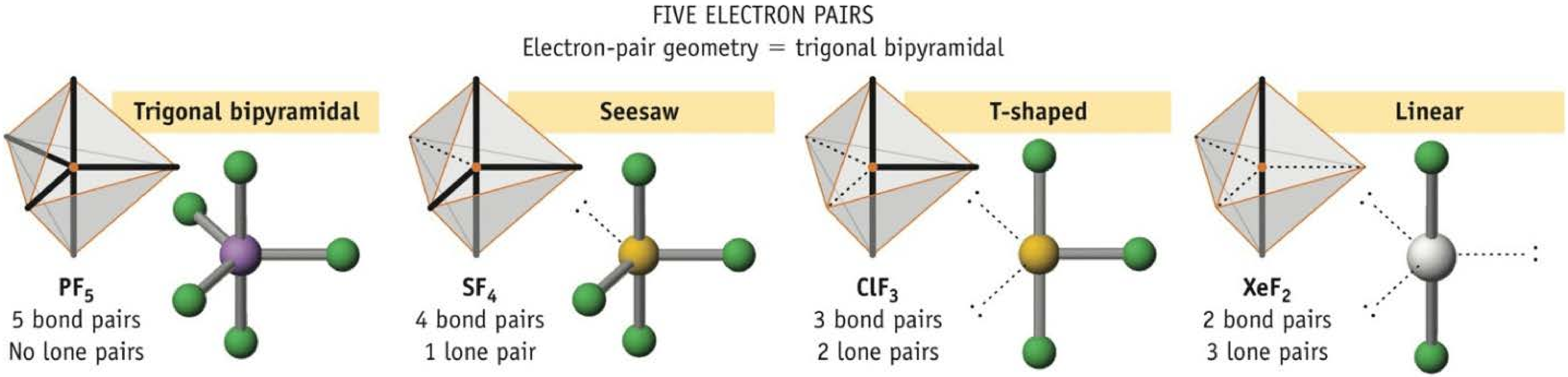
SO_2

Electronic Geometry: Tetrahedral (SN=4)

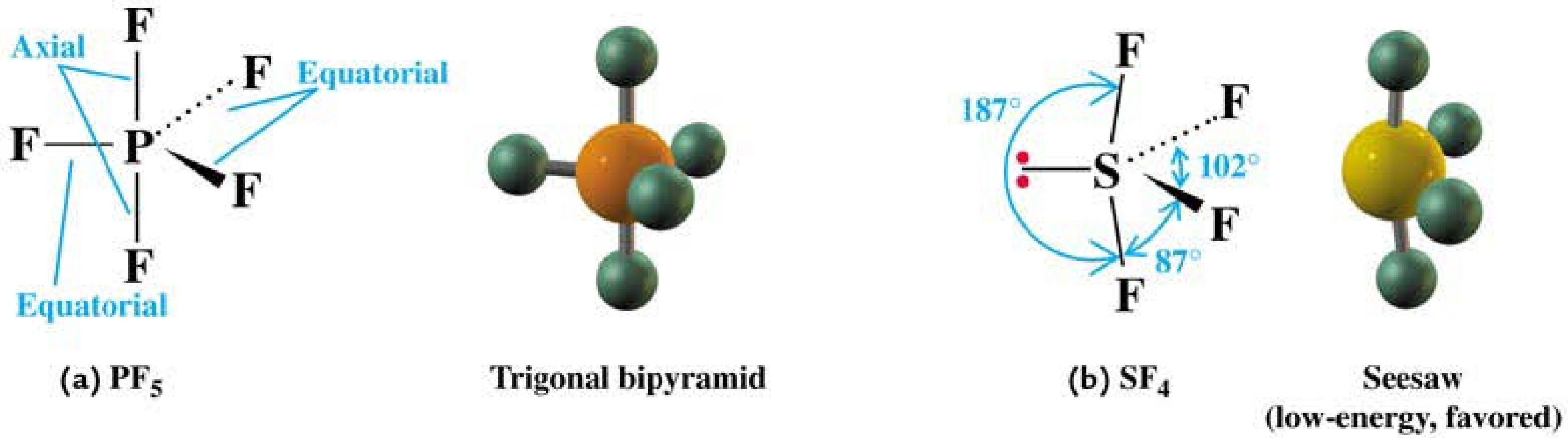


Electronic Geometry: Trigonal Bipyramidal (SN=5)

5) valence shell expansion (VSE)

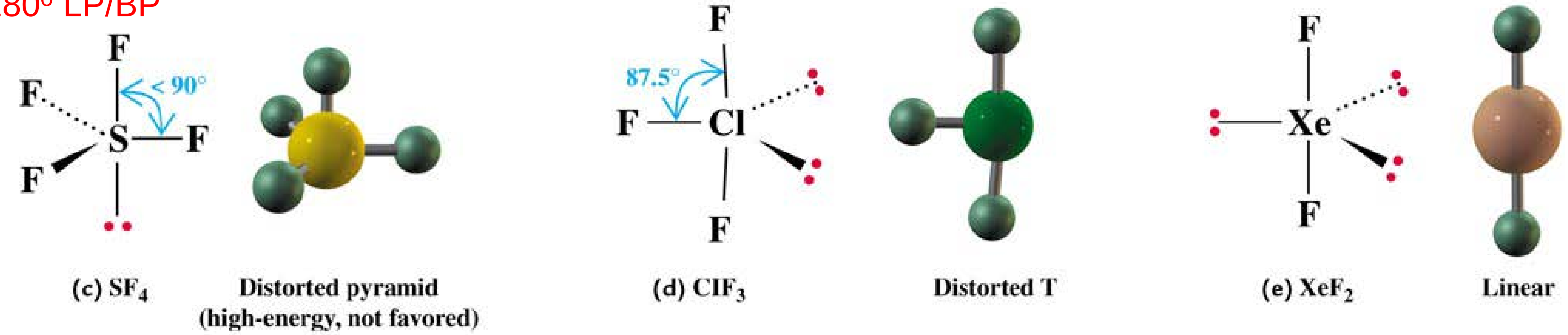


Trigonal Bipyramidal: Where are LP Electrons?

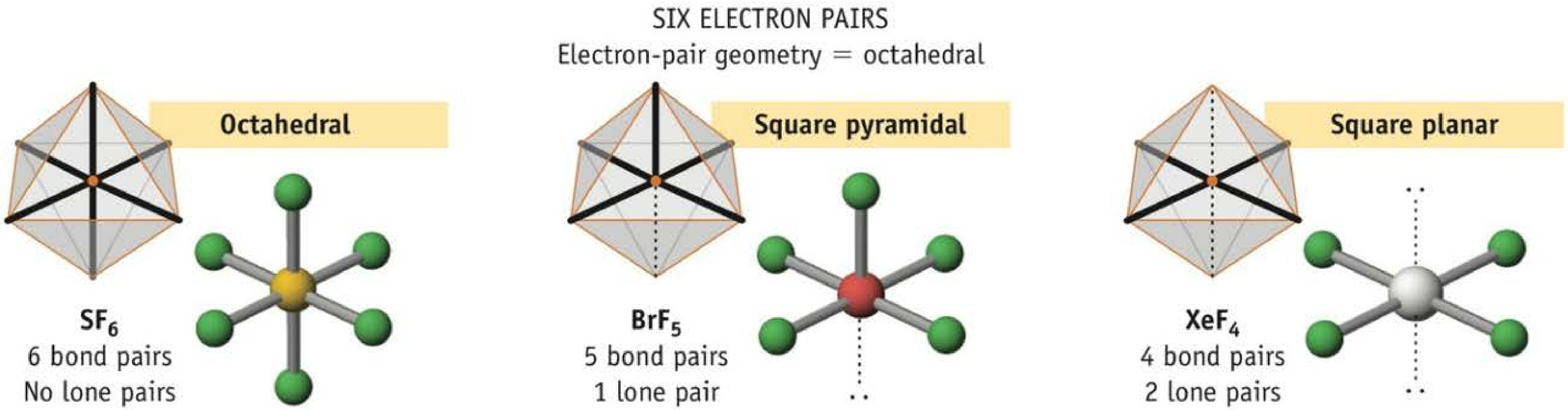


2 90º LP/BP
2 120º LP/BP

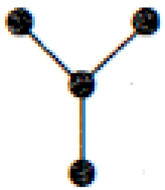
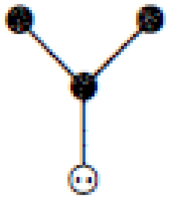
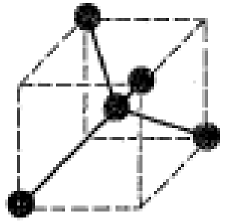
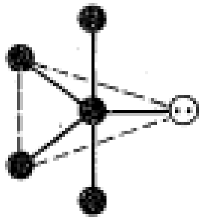
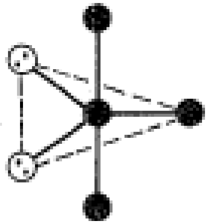
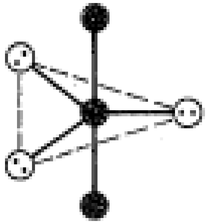
3 90º LP/BP
1 180º LP/BP



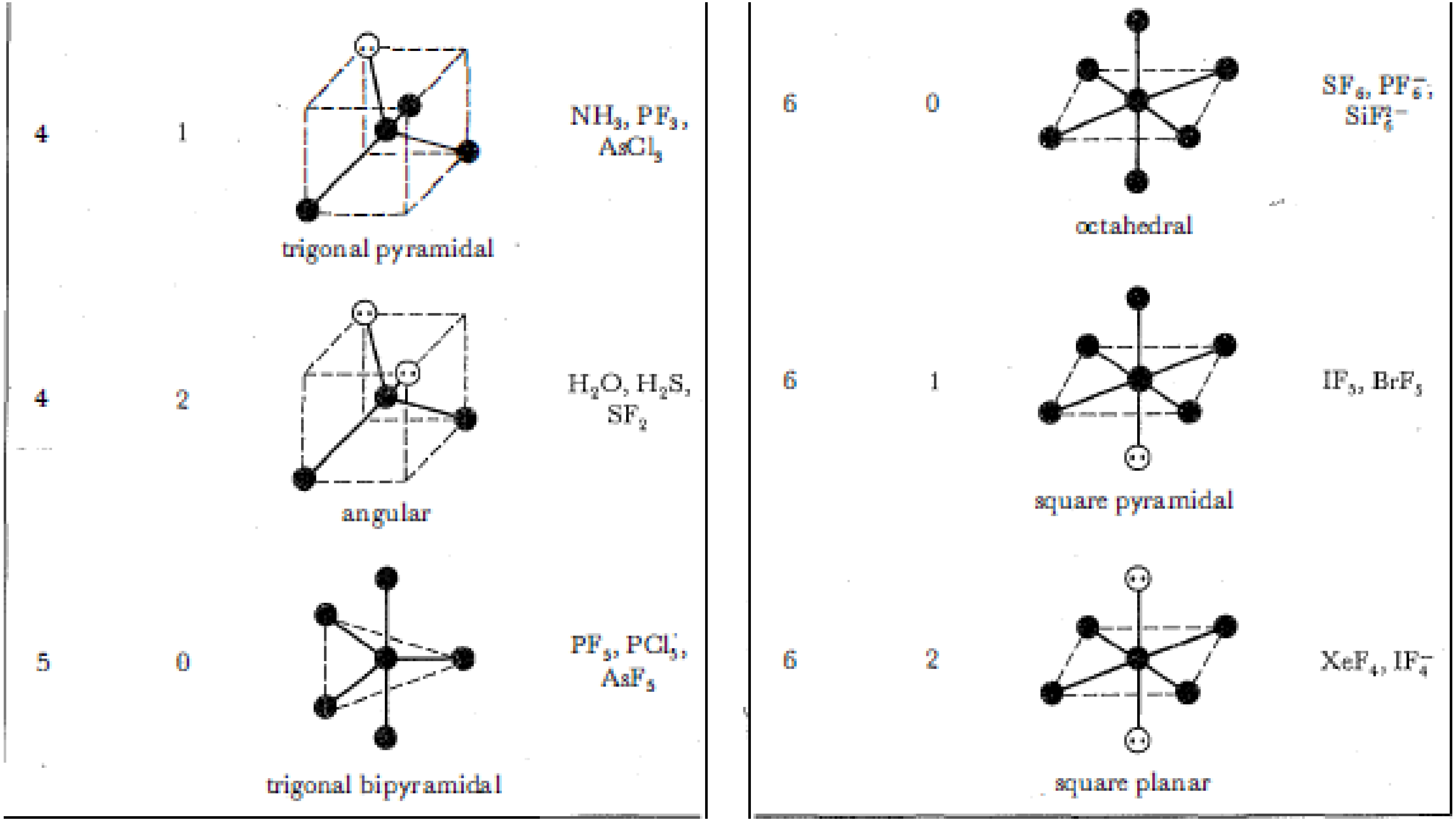
Electronic Geometry: Octahedral (SN=6)



Lewis Structures and VSEPR

SN	Number of lone pairs	Molecular shape	Example
2	0	 linear	BeH_2, CO_2
3	0	 trigonal planar	SO_3, BF_3
3	1	 angular	SO_2, O_3
4	0	 tetrahedral	CH_4, CF_4, SO_4^{2-}
5	1	 sawhorse	SF_4
5	2	 T-shaped	ClF_3
5	3	 linear	XeF_2, I_3^-, IF_2^-

Lewis Structures and VSEPR (Beyond Octets)



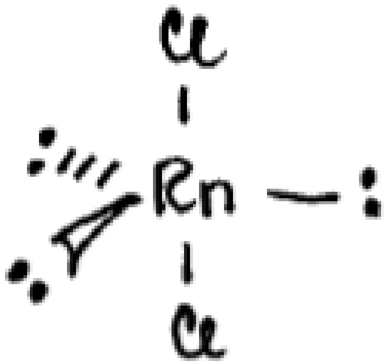
5) VSE (Valence Shell Expansion)

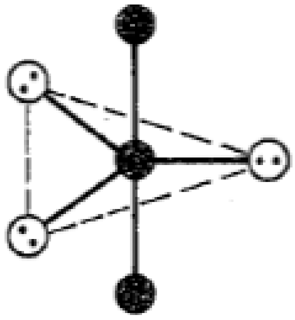
$RnCl_2$

VAL = 8 + 2(7) = 22
STAB = 3(8) = 24
BOND = 24 – 22 = 2/2 = 1 BP
LONE = 22 – 2 = 20/2 = 10 LP
2 Rn – Cl bonds => VSE =>
  2 BP, 9 LP (6 on Cl)

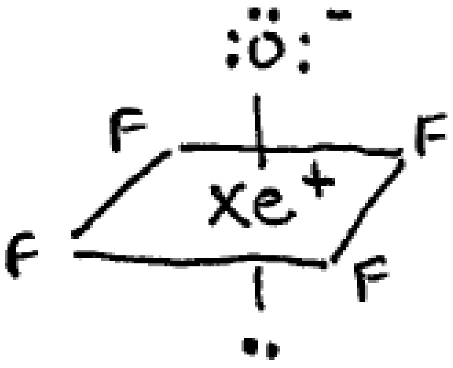
$XeOF_4$

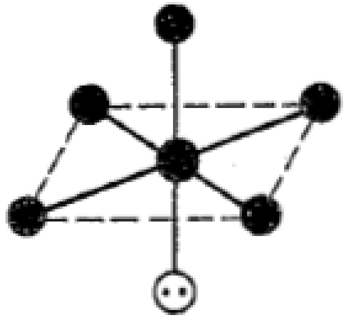
VAL = 8 + 6 + 4(7) = 42
STAB = 6(8) = 48
BOND = 48 – 42 = 6/2 = 3 BP
LONE = 42 – 6 = 36/2 = 18 LP
need 5 bonds => 5 BP => 2 VSE expansions
  5 BP, 16 LP (15 on O,F)





linear





square pyramidal

1A (1)	2A (2)	3B (3)	4B (4)	5B (5)	6B (6)	7B (7)	(8)	8B (9)	(10)	1B (11)	2B (12)	3A (13)	4A (14)	5A (15)	6A (16)	7A (17)	8A (18)
1 **H** 1.008																	2 **He** 4.0026
3 **Li** 6.94	4 **Be** 9.0122											5 **B** 10.81	6 **C** 12.011	7 **N** 14.007	8 **O** 15.999	9 **F** 18.998	10 **Ne** 20.180
11 **Na** 22.990	12 **Mg** 24.305											13 **Al** 26.982	14 **Si** 28.085	15 **P** 30.974	16 **S** 32.06	17 **Cl** 35.45	18 **Ar** 39.95
19 **K** 39.098	20 **Ca** 40.08	21 **Sc** 44.956	22 **Ti** 47.867	23 **V** 50.942	24 **Cr** 51.996	25 **Mn** 54.938	26 **Fe** 55.85	27 **Co** 58.933	28 **Ni** 58.693	29 **Cu** 63.55	30 **Zn** 65.4	31 **Ga** 69.723	32 **Ge** 72.63	33 **As** 74.922	34 **Se** 78.97	35 **Br** 79.904	36 **Kr** 83.80
37 **Rb** 85.468	38 **Sr** 87.62	39 **Y** 88.906	40 **Zr** 91.22	41 **Nb** 92.906	42 **Mo** 95.95	43 **Tc** (97/8)	44 **Ru** 101.1	45 **Rh** 102.91	46 **Pd** 106.42	47 **Ag** 107.87	48 **Cd** 112.41	49 **In** 114.82	50 **Sn** 118.71	51 **Sb** 121.76	52 **Te** 127.6	53 **I** 126.90	54 **Xe** 131.29
55 **Cs** 132.91	56 **Ba** 137.33	57 **La** 138.91	72 **Hf** 178.5	73 **Ta** 180.95	74 **W** 183.84	75 **Re** 186.21	76 **Os** 190.2	77 **Ir** 192.22	78 **Pt** 195.08	79 **Au** 196.97	80 **Hg** 200.59	81 **Tl** 204.38	82 **Pb** 207.2	83 **Bi** 208.98	84 **Po** (209)	85 **At** (210)	86 **Rn** (222)
87 **Fr** (223)	88 **Ra** (226)	89 **Ac** (227)	104 **Rf** (267)	105 **Db** (268)	106 **Sg** (269)	107 **Bh** (271)	108 **Hs** (277)	109 **Mt** (276/7)	110 **Ds** (281)	111 **Rg** (282)	112 **Cn** (285)	113 **Nh** (286)	114 **Fl** (289)	115 **Mc** (290)	116 **Lv** (293)	117 **Ts** (294)	118 **Og** (294)

Lanthanides	58 **Ce** 140.12	59 **Pr** 140.91	60 **Nd** 144.24	61 **Pm** (145)	62 **Sm** 150.4	63 **Eu** 151.96	64 **Gd** 157.3	65 **Tb** 158.93	66 **Dy** 162.50	67 **Ho** 164.93	68 **Er** 167.26	69 **Tm** 168.93	70 **Yb** 173.05	71 **Lu** 174.97
Actinides	90 **Th** 232.04	91 **Pa** 231.04	92 **U** 238.03	93 **Np** (237)	94 **Pu** (244)	95 **Am** (243)	96 **Cm** (247)	97 **Bk** (247)	98 **Cf** (251)	99 **Es** (252)	100 **Fm** (257)	101 **Md** (258)	102 **No** (259)	103 **Lr** (262)