VSEPR THEORY AND SHAPES OF MOLECULES

There is a very simple theory that is remarkably effective in predicting the shapes of molecules formed by the representative elements. The **Valence Shell Electron Pair Repulsion Theory (VSEPR Theory)** is based on the idea that valence shell electron pairs stay as far apart as possible from each other to minimize the repulsions between them.

EXAMPLE	No. Bonding Electron Pairs on Central Atom	No. Lone Pairs of Electrons on Central Atom	VSEPR Shape and Formula	Model, Example and Bond Angles
$BeCl_2$				
BCl_3				
CN^{-1}				
CH_2Cl_2				
HCHO				
CH_4				
NH_3				
H_2O				

NOTE: The last 2 shapes (trigonal pyramidal and bent) are simply variations on the tetrahedral. **ALL** three of these shapes require a **TOTAL** of 4 pairs of electrons around the central atom.

Other VSEPR shapes to know:

EXAMPLE	No. Bonding Electron Pairs on Central Atom	No. Lone Pairs of Electrons on Central Atom	VSEPR Shape and Formula	Model, Example and Bond Angles
PCl_5				
SF_4				
ClF_3				
SF_6				
BrF_5				
XeF_4				
I_3^{1-}				
$HCOO^{-1}$				
SO_3^{-2}				
TeF_2				

Assignment:

1. The molecules NF_3, BF_3, and ClF_3 all have molecular formulas of the type XF_3, but the molecules have different molecular geometries. Predict the shape of each molecule and explain the origin of the differing shapes.

2. The molecules SiF_4, SF_4, and XeF_4 all have molecular formulas of the type XF_4, but the molecules have different molecular geometries. Predict the shape of each molecule and explain the origin of the differing shapes.

3. The three species NO_2^+, NO_2, and NO_2^{-1} all have a central nitrogen atom. The ONO bond angles in the three species are 180^0, 134^0, and 115^0, respectively. Explain this variation in bond angles.

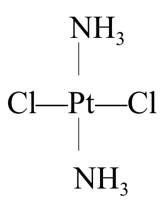
4. The three species NH_2^{-1}, NH_3, and NH_4^{+1} have H — N — H bond angles of 105^0, 107^0, and 109^0 respectively. Explain this variation in bonds angles.

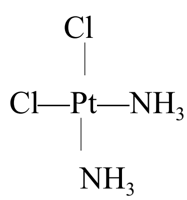
5. Despite the larger electronegativity difference between the bonded atoms, $BeCl_{2(g)}$ has no dipole moment whereas $SCl_{2(g)}$ does possess one. Account for this difference in polarity,

6. The PF_3 molecule has a dipole moment of 1.03 D, but BF_3 has dipole moment of zero. How can you explain the difference.

7. The H — P — H bond angle in PH_3 is 93^0; in PH_4^{+1} it is 109.5^0. Account for this difference.

8. There are two compounds of the formula $Pt(NH_3)_2Cl_2$:





The compound on the right, known as *cisplatin*, is used in cancer therapy. Both compounds have a square planar geometry. Which compound have a nonzero dipole moment?

9. The nitrogen-nitrogen bond lengths in N_2H_4, N_2F_2, and N_2 are 1.45, 1.25, and 1.10 Å, respectively. How can this trend be explained?

10. Predict the molecular geometry of:
    (a) AsF_3
    (b) OCN^{-1}
    (c) H_2CO
    (d) NCS^{-1}
    (e) HCO(OH) which has an H and two O atoms attached to C.