NOTES #28 Bonds & Thermochemistry AP Chemistry

- When studying thermochemistry, we determined $\Delta H°$ or ΔH_{rxn} of a reaction by using $\Delta H°f$ values. For practice's sake, determine ΔH_{rxn} for the formation of water according to the following rxn: ($\Delta H°f$ (H_2O) = -241.8 kJ/mol)

$$2\ H_2\ (g) + O_2\ (g) \rightarrow 2\ H_2O\ (g)$$

- Instead of looking at the total heat released to form a certain compound, we can also predict $\Delta H°$ by looking at the energies associated with each BOND in a certain compound. It's the BONDS, after all, that are made or broken that determine the stability of the compounds and whether the reaction is endothermic or exothermic.

A. Bond Dissociation Energy

1. What is it? The enthalpy change required to <u>break</u> one particular bond in 1 mole of gaseous molecules. Breaking bonds is always an _____ process.

** The MORE energy it takes to break a bond (greater bond energy), the _____ stable the bond.

Ex. H-H (g) → H (g) + H (g) $\Delta H°$ = 436.4 kJ
Cl-Cl (g) → Cl (g) + Cl (g) $\Delta H°$ = 242.2 kJ

2. Except for in diatomic molecules (like the ones above), bond dissociation energies are AVERAGED values because bond energies are affected by their environment. ALL O-H bonds, for example, do not have the same energy. For example,

a. The energy needed to break the 1st O-H bond in H_2O is different from the energy needed to break the 2nd O-H bond:

H_2O (g) → H (g) + O-H (g) $\Delta H°$ = 502 kJ
O-H (g) → H (g) + O (g) $\Delta H°$ = 427 kJ

b. The energy to break O-H bonds in two different molecules is different
CH_3OH (g) → CH_3O (g) + H (g) $\Delta H°$ = 477 kJ
H_2O (g) → H (g) + O-H (g) $\Delta H°$ = 502 kJ

** Scientists measure the heat required to break an O-H bond in a number of different situations and take the average to get the bond dissociation constants you see in your book.

3. Single bonds have _____ energy than double bonds which have _____ energy than triple bonds.
(C-C 347 kJ; C=C 620 kJ ; C≡C 812 kJ)

So, which type of bond is the STRONGEST? _____ It requires the most energy to be broken.

B. Determining $\Delta H°$ from bond energies

1. BOND BREAKING = _____ ENERGY = REACTANTS
BOND FORMING = _____ ENERGY = PRODUCTS

2. $\Delta H°$ = total energy input (bonds broken) - total energy released (bonds formed) **or**

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3. Example: Calculate the enthalpy change for the combustion of hydrogen gas using bond energies
(H-H 436.4 kJ ; O=O 498.7 kJ ; O-H 460 kJ)

$2\ H_2\ (g) + O_2\ (g) \longrightarrow 2\ H_2O\ (g)$

** Compare your ΔH_{rxn} values. Which value do you think is more reliable and why????

Practice Problems:

1. A) Determine the ΔH_{rxn} using bond energies:

$2\ C_2H_6(g) + 7\ O_2(g) \longrightarrow 4\ CO_2(g) + 6\ H_2O(g)$

Bond Energies (kJ/mol)
C-H = 414
C-C = 347
O=O = 498.7
C=O = 799
O-H = 460

B) Determine the ΔH_{rxn} using $\Delta H°f$ values:

$\Delta H°f$ values in kJ/mol
$CO_2(g)$ = -393.5
$H_2O(g)$ = -241.8
$C_2H_6(g)$ = -87.4

2. Determine the ΔH_{rxn} using bond energies:

$CH_4(g) + 2\ Cl_2(g) + 2\ F_2(g) \longrightarrow CF_2Cl_2(g) + 2\ HF(g) + 2\ HCl(g)$
freon

Bond Energies in kJ/mol
C-H = 414
Cl-Cl = 242.7
F-F = 156.9
C-F = 485
C-Cl = 339
H-F = 565
H-Cl = 42

NOTES #29 Dipole Moments/Molecular Polarity/Hybridization

A. **BOND POLARITIES:** You learned about bonds being polar or non-polar depending on the _____differences of the atoms. What is ELECTRONEGATIVITY?

* An example of a polar bond is _____.

* An example of a non-polar bond is _____.

B. **MOLECULE POLARITIES:** Now, we are going to look at an entire molecule and decide if the *molecule* itself is polar or not. If a molecule is POLAR it is said to have a DIPOLE or a dipole moment, meaning the molecule itself has a partial (+) end and a partial (-) end. Just because a molecule has polar bonds doesn't necessarily mean that it will be a polar molecule. There are THREE general rules for determining the polarity of a molecule.

1. A molecule that is symmetrical is _____ , but this is only true if all of the bonds are identical.
It does not matter how polar the individual bonds are. EX:

2. An asymmetrical molecule is POLAR as long as the bonds are polar as well.
A central atom with lone pairs is *often* asymmetrical. EX:

3. A molecule with more than one type of atom attached to the central atom is *often* (not always) asymmetrical and therefore _____.

** Sometimes, you might be asked to indicate the DIRECTION of the dipole. Just like with polar bonds, the dipole always points towards where the partial _____end is.

Examples: Draw each molecule and determine if it is polar or non polar. If polar, try to indicate the direction of the dipole.

a) $SiCl_4$ b) CH_2Cl_2 c) NH_3 vs NF_3

d) CO_2 e) SF_4 f) XeF_4

e) $Cl_2C_2H_2$

Why is this important? Polarity (or lack of polarity) determines many physical/chemical characteristics of a molecule.

1. For example, POLAR substances dissolve in POLAR substances and NON POLAR substances dissolve in NON-POLAR substances. In other words, "like dissolves like." EX: VITAMINS

2. Polar substances, since they have partial charges, conduct electricity better. DEMO

HYBRIDIZATION

A. **INTRO:** We've been drawing all these structures but what has to happen on an orbital level to make it all happen????

a) Illustrate how H-H would bond?

b) Illustrate how Cl-Cl would bond?

c) Not all bonding is so simple. Let's take an *orbital* look at methane, CH_4.

- Draw C's orbital diagram: [He] _____ (2s) ____ ____ ____ (2p)

** What do we have to do to accommodate ALL 4 H's??

** Now, we can bond all the H's, but think of what this molecule would actually look like remembering the orientations of the different orbitals.

- *NEW*, excited orbital diagram of C: _____ (2s) ____ ____ ____ (2p)

B. HYBRIDIZATION: when at least two different types of orbitals of the same atom mix to make NEW, equivalent orbitals which will allow covalent bond formation.

** We would say that the C in methane is _____ hybridized and bonds using _____ hybrid orbitals.

** NOTE that the number of hybrid orbitals generated is EQUAL to the number of pure atomic orbitals that participate in the hybridization process. We mixed _____ pure orbitals and made _____ hybrid orbitals.

C. Let's look at another example. What hybridization does B have in the compound BH_3?

- Look at B's orbital diagram: (3 valence electrons)

** This is an example of _____ hybridization

NOTES #30 HYBRIDIZATION CONTINUES/MULTIPLE BONDS

D. Other examples. Specify the hybridization of the underlined central atom in each example below.

a. <u>Be</u>Cl2

b. <u>P</u>Cl5

c. <u>S</u>F6

E. Summary of things to know:

1. The concept or hybridization is not applied to isolated atoms. It's a theoretical model used ONLY to explain covalent bonding.

2. Hybridization requires an input of energy (especially when an electron is promoted to higher energy levels); However, the system more than recovers this energy during bond formation (Remember, bond formation ALWAYS releases energy).

** 3. The number of hybrid orbitals generated is ALWAYS equal to the number of pure atomic orbitals that participated in the hybridization process.

** 4. If you know the number of <u>total number of electron domains</u>, you can easily determine the hybridization of the central atom. What is an electron domain?

# of electron domains	Geometry	hybridization
2	linear	sp (s + p)
3	trigonal planar	sp^2 (s + p + p)
4	tetrahedral	sp^3 (s + p + p + p)
5	trigonal bipyramidal	sp^3d (s + p + P + P + d)
6	octahedral	sp^3d^2 (s + p + p + p + d + d)

** Remember, "electron domains" include BOTH bonding pairs and lone pairs!!! And, double or triple bonds are counted as just 1 single electron domain. In other words, you are really just counting *protrusions* or concentrated electron extensions from the central atom....

*** Determine the hybridization of the following molecules. ***

a) PH3 b) H2S c) CO32- d) SF5- e) SF4

F. More on hybridization in molecules containing double and triple bonds.

1. Let's look at ethylene, C_2H_4. We know the C's in C_2H_4 are _____ hybridized. How can we explain that looking at the orbitals?

2. This introduces two types of covalent bonds:
   - **sigma bond** (σ bond) - end-to-end bonds; e- density concentrated between the nuclei of the bonding atoms.
   - **pi bond** (π bond) - sideways overlapping bonds; e- density concentrated above and below the plane of the nuclei of the bonding atoms. *Pi bonds always form from UNHYBRIDIZED p ORBITALS!!*

   * A SINGLE bond is always a _____ bond.
   * A DOUBLE bond is always a _____ bond and a _____ bond.
   * A TRIPLE bond is always a _____bond and TWO _____ bonds. Take a look....

3. Let's look at acetylene molecule, C_2H_2

4. You need to be able to look at a molecule and identify all of the sigma bonds and pi bonds:

   Ex.

G. DELOCALIZATION: another look at resonance...