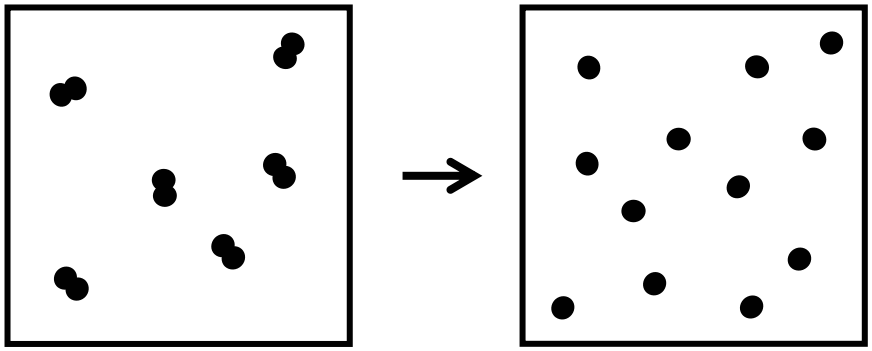
CHM 101 Project #3 Name_____
Sinex

Reaction Dynamics: The Energetics

Let's consider a simple reaction using the "molecules in the box" approach and the energy involved in chemical bonds. Are bonds breaking or forming for the boxes below?



The example above illustrates the dissociation of a diatomic molecule into atoms and the process requires energy to be added.

$$\text{energy} + Cl_2\,(g) \rightarrow 2Cl\,(g)$$

The energy needed to break a mole of Cl-Cl bonds is the bond energy. The bond energies for diatomic halogen molecules with single bonds are given in the table below. Draw a Lewis dot structure of one of the halogens to verify the single bond.

| Molecules | Bond Energy |
|---|---|
| $F_2$ | 154 kJ/mole |
| $Cl_2$ | 239 |
| $Br_2$ | 193 |
| $I_2$ | 149 |

Zumdahl and Zumdahl (2003) *Chemistry*, 6th ed.

Which halogen molecule is easiest to dissociate? Why?

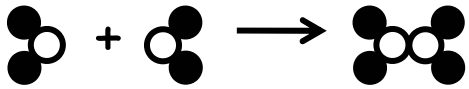
If you placed 2.0 moles of fluorine atoms in a container, you would find, after a period of time, 1.0 mole of $F_2$ molecules. Would energy be required or released in this reverse reaction, where bonds are formed? Explain.

When energy is absorbed in a process or reaction, it is referred to as endothermic process or reaction. While when energy is released, it is an exothermic process or reaction. We can use average bond energies to estimate the amount of energy absorbed or released in a reaction.

| Process | Endothermic or exothermic |
|---|---|
| Bond breaking | |
| Bond forming | |

Is the dimerization of $NO_2$, endothermic or exothermic? Why?

$$2NO_2\ (g) \rightarrow N_2O_4\ (g)$$



Draw a Lewis dot structure of $N_2O_4$. What type of nitrogen-nitrogen bond forms?

Now let's consider a more involved reaction as given below. With the help of Lewis dot structures, what types of bonds and how many are broken and formed? List them and using your textbook, look up their bond energies. Add up the total energy for the bonds broken and compare to the total for the bonds formed.

$$H_2\ (g) + Cl_2\ (g) \rightarrow 2HCl\ (g)$$

Which side of the reaction (reactants or products) involves the larger amount of energy?

Is this reaction endothermic or exothermic? Why?

Is the synthesis of ammonia from its elements an endothermic or exothermic reaction? With the help of Lewis dot structures, what types of bonds and how many are broken and formed? List them and using your textbook, look up their bond energies.

$$N_2\,(g) + 3H_2\,(g) \rightarrow 2NH_3\,(g)$$

This is a simple exercise in bookkeeping all the bonds broken and formed. The heat of reaction, $\Delta H$, is calculated by the equation below, where BE is the bond energy.

$$\Delta H = \sum \text{BE (bonds broken)} - \sum \text{BE (bonds formed)}$$

What is the sign of $\Delta H$ for an endothermic reaction?

What is the sign of $\Delta H$ for an exothermic reaction?

Go to http://academic.pgcc.edu/~ssinex/chm101.html and find the "Bond Energy Calculator," an interactive Excel spreadsheet that will do the calculations with the bookkeeping input and energies. Remember this is estimating $\Delta H$.

Using Lewis dot structures to determine bond type (single, double, or triple) and average bond energies from your textbook, calculate the value of $\Delta H$ and determine if the following reactions are endothermic or exothermic.

$$CH_4\,(g) + 2O_2\,(g) \rightarrow CO_2\,(g) + 2H_2O\,(g)$$

$$H_2O\,(g) \rightarrow 2H\,(g) + O\,(g)$$

$$CH_4\,(g) + 2Cl_2\,(g) + 2F_2\,(g) \rightarrow CF_2Cl_2\,(g) + 2HF\,(g) + 2HCl\,(g)$$

Explain these two general observations:

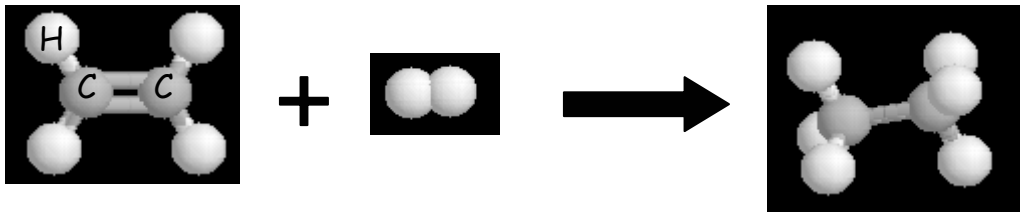
1. Acid-base neutralization reactions tend to be exothermic.

$$H^+ + OH^- \rightarrow H_2O$$

2. Weak acid dissociation reactions, such as HCN shown below, tend to be endothermic.

$$HCN \rightarrow H^+ + CN^-$$

Consider the gas-phase reaction for the addition of $H_2$ to ethene, $C_2H_4$, given below. Do all the bonds need to be broken and then formed? *Describe* the actual bond breaking and forming needed for this reaction.




| $C_2H_4$ | $H_2$ | $C_2H_6$ |
|---|---|---|
| $H_2C{=}CH_2$ | H-H | $H_3C\text{-}CH_3$ |

This reaction is the basis for hydrogenation (adding $H_2$ across double bonds) of vegetable oils (liquids) to form Crisco vegetable shortening and margarines (solids).