Chem 30 **Thermochemistry**

Thermochemistry is the study of chemical changes and the energy associated with the change.

Energy is the ability to do work; create heat and/or generate electricity. Energy can exist in many different forms, but is classified into two main types: potential energy and kinetic energy.

* Chemical *potential energy* relates to the attractions between atoms and molecules. When a chemical or phase change occurs, atoms or molecules are rearranged and new attractions are made. The change in the attractions contributes to the energy associated with the change.
* *Kinetic energy* (Ek) is the energy due to the motion of particles. There are three types of motion vibrational, translational, and rotational.

Both types of energies can be demonstrated on graphs.

Kinetic energy is shown by a **heating or cooling curve**:

Graph A

bp

Temperature

or Ek (oC)

mp

Time

**Potential energy diagrams** are graphs that show the change in energy due to the change:

Graph B

H2O(l)

Ep Heat

(joules) H2O(s)

Time

**Energy changes** can be described as endothermic; absorbing heat or exothermic; releasing heat.

Thermal energy is the sum of all Ek and Ep added together. Heat is only the energy that is transferring from one substance to another. Temperature is a measure of only the kinetic energy of a substance. Potential energy is not directly measurable.

Heat capacity is the amount of heat that a substance can absorb before it’s temperature rises one degree. (Units are J/oC) Specific heat capacity (c) is the amount of heat that **one gram** of a substance can absorb before its temperature rises one degree. (Units are J/goC)

\*The specific heat for water is 4.19 J/goC

The three types of potential changes that occur are:

**Phase changes**; the state of the substance changes by either gaining or losing energy. The amount of energy is usually in the 10’s to 100 KJ. Energy from phase changes are typically due to changes in intermolecular forces.

**Chemical changes**; a new substance with new properties is produced. The bonds between atoms are changed. Usually the amount of energy is in the 1000’s of KJ.

**Nuclear changes**; an entirely new element is formed. Attractions within the nucleus are affected. Energy of these changes is often in the 1,000,000’s of KJ

*Diagram A*

**O** Interatomic bonds

**O H H**

**H H**

Intermolecur forces

**O**

**H H**

**Calculating heat**

There are three factors that affect the amount of heat within a substance: the mass of the substance, the specific heat capacity of the substance, and the change in the temperature.

We can use these to produce the formula:

H = mc t

“Change in heat equals mass times specific heat capacity times change in temperature”

**Calorimetry**

This is an experimental method of measuring heat transfer.

* A calorimeter is ideally an isolated system, so no energy is lost or gained by the environment.
* The first law of thermodynamics is that heat cannot be created or destroyed but can be transferred from one substance to another.
* The second law of thermodynamics is that heat naturally flows from a warm object to a cooler one until equilibrium is reached.

Using the three principles from above we can state that any heat lost from one substance in a calorimeter must be equal to the heat gained by another substance in the calorimeter.

Most calorimetry problems involve calculating the heat of water in the calorimeter and saying it is equal to the heat change of another substance in the calorimeter. This allows us to calculate heats of potential form as long as the heat is transferred to a kinetic form. In a calorimeter a thermometer can measure temperature change which can be used to calculate heat.

Eg. A piece of molten metal is dropped into a calorimeter filled with 500 ml of water. The water warms 11.8oC when the metal solidifies. How much heat does the metal release when freezing (solidifying)?

***Molar heat ( H )***

The heat associated with **one mole** of a substance changing. H= h/n Units are KJ/mol.

It is possible to calculate a molar heat for any type of change.

***Molar heats of formation ( Hf )***

This is the amount of heat, usually released, associated with a simple composition reaction, also known as a formation reaction. “The amount associated with the production of one mole of a substance from it’s elements.”

***Additivity***

All reactions are the rearrangement of valence electrons to form new bonds. In most reactions bonds of the reactant molecules are broken which requires heat (endothermic) and then the new bonds for products are formed which releases heat (exothermic).

Large changes can be thought of as a series of simple decomposition and the simple composition reactions. The heats related to formation reactions have been calorimetrically determined and tabled in data booklets. We can use additivity to predict the heats for more complex changes.

Eg. CH4 + 2O2  🡺 CO2 + 2H2O

CH4 🡺 C + 2H2  - H*f* = 74.6 KJ/mol x 1 mol

C + O2 🡺 CO2  H*f* = -393.5 KJ/mol x 1 mol

2H2 + O2  🡺 2H2O H*f* = -241.8 KJ/mol x 2 mol

\*\*\* Any reactions that are added together produce a net change that has a heat equal to the sum of the heats of the reactions that are added together. Sometimes we reverse reactions, changing the sign of their heat value, sometimes we multiply the reaction and its heat value by a factor. Adjust whatever is necessary to produce the desired sum for the given reactions.

**Hess’ Law**

Using the idea of additivity we can simplify the calculations to the following equation:

ΔHrxn = ∑H*f* reactants x n - ∑H*f* products x n

\*\*\*There are many heat calculation problems

**Collision theory**

Reaction progress is dependent on many factors. Two of the main factors affecting the rate of a reaction are: - The number of collisions that occur.

- The energy of the collision.

**More collisions** with **more energy** involved will increase the probability that the reaction occurs. The probability of a reaction occurring depends on the *number of particles*, the *speed of particles*, *how they collide*, etc.

Activation energy is an energy barrier that must be overcome before a reaction will occur.

Activated complex is and intermediate chemical entity composed of the collided reactants.

The energy within any bond is unique. The amount of energy associated with a specific bond will determine the collision energy required to cause a reaction to occur.

A **catalyst** is a substance or process that increases the rate of a reaction without being consumed itself by the reaction. Catalyzed reactions will have lower activation energy pathways than normal.

**Intermediates** are substances that form as an interim during a chemical change. They are more stable than the activated complex but less stable than the products or reactants.

Uses of catalysts include oil refining and enzymes.