Name: **Thermochemistry Notes**

**I. Thermochemistry** deals with the changes in energy that accompany a chemical reaction. Energy is measured in a quantity called enthalpy, represented as H. The change in energy that accompanies a chemical reaction is represented as ΔH. Page 519

a. The energy absorbed or released as heat in a chemical or physical change is measured in a **calorimeter**. In one kind of calorimeter, known quantities of reactants are sealed in a reaction chamber, which is immersed in a known quantity of water in an insulated vessel. Therefore, the energy given off (or absorbed) during the reaction is equal to the energy absorbed (or given off) by the known quantity of water. The amount of energy is determined from the temperature change of the known mass of surrounding water.

Using the change in temperature, ΔT, determined from calorimeter one can use the following equation to determine the quantity of energy gained or lost during the reaction or for a physical change:

|  |  |
| --- | --- |
| **Substance** | **Specific heat J/(g•K)** |
| Water (l) | 4.18 |
| Ethanol (l) | 2.44 |
| Aluminum (s) | 0.897 |
| Copper (s) | 0.385 |
| Gold (s) | 0.129 |
| Iron (s) | 0.449 |

q = (cp)(m)(ΔT)

ΔT in kelvin

q represents the energy lost or gained (in J)

m is the mass of the sample (in g)

cp is the specific heat of a substance at a given temperature

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Practice Problem: 1. How much heat energy is needed to raise the temperature of a 33.0 gram sample of aluminum from 24.0°C to 100.°C?

2. Determine the specific heat of a material if a 35 g sample absorbed 96 J as it was heated from 293K to 313K.

3. During a chemical reaction carried out in a calorimeter the temperature of water within the calorimeter raised from 24.0°C to 125°C. If 250. grams of water were present calculate the amount of heat energy the water gained.

b. In **thermochemical equations** the quantity of energy released or absorbed as heat during a reaction is written and is represented by ΔH.

Example: 2H2(g) + O2(g) → 2H2O(l) ΔH= - 571.6 kJ/mol

c. ΔH can be used to determine if the reaction is exothermic or endothermic. If the ΔH value of an equation is **negative that represents an exothermic reaction**. (Meaning energy is released, therefore the energy of the products would be less.)

If the ΔH value of an equation is **positive that represents an endothermic reaction**. Example:

2H2(g) + O2(g) → 2H2O(g) ΔH= - 483.6 kJ/mol Type of Reaction: Exothermic

ΔH reactants = 1450.8 kJ/mol

ΔH products = 967.2 kJ/mol

2H2O(g) → 2H2(g) + O2(g) ΔH= + 483.6 kJ/mol Type of Reaction: Endothermic

ΔH reactants = 967.2 kJ/mol

ΔH products = 1450.8 kJ/mol

d. Hess’s law provides a method for calculating the ΔH of a reaction from tabulated data. This law states that if two or more chemical equations are added, the ΔH of the individual equations may also be added to find the ΔH of the final equation. As an example of how this law operates, look at the three reactions below.

|  |  |  |
| --- | --- | --- |
| (1) | 2H2(g) + O2(g) → 2H2O(l) | ΔH = −571.6 kJ/mol |
| (2) | 2H2O2(l) → 2H2(g) + 2O2(g) | ΔH = +375.6 kJ/mol |
| (3) | 2H2O2(l) → 2H2O(l) + O2(g) | ΔH = ? kJ/mol |

When adding equations 1 and 2, the 2 mol of H2(g) will cancel each other out, while only 1 mol of O2(g) will cancel.

|  |  |  |
| --- | --- | --- |
| (1) + (2) | ~~2H~~~~2~~~~(g)~~ + O2(g) + 2H2O2(l) → 2H2O(l) + ~~2H~~~~2~~~~(g)~~ + 2O2(g) | ΔH = (−571.6 kJ/mol)  + (+375.6 kJ/mol) |
| (3) | 2H2O2(l) → 2H2O(l) + O2(g) | ΔH = ? kJ/mol |

Notice the combined equation is the same as equation 3. Adding the two ΔH values for the reactions 1 and 2 gives the ΔH value for reaction 3. Using Hess’s law to calculate the enthalpy of this reaction, the following answer is obtained.

−571.6 kJ/mol + 375.6 kJ/mol = −196.0 kJ/mol

Thus, the **ΔH value** for the reaction is **−196.0 kJ/mol** and is an **exothermic reaction** because it is negative!

Practice Problem 4: Use equations 1, 2, and 3 below to calculate the ΔH values for equation 4 (the formation of methane). Is reaction 4 exothermic or endothermic?

|  |  |  |
| --- | --- | --- |
| (1) | C(s) + O2(g) → CO2(g) | ΔHf = −393.5 kJ/mol |
| (2) | CH4(g) + 2O2(g) → CO2(g) + 2H2O(l) | ΔHc = −890.8 kJ/mol |
| (3) | H2(g) + ½ O2(g) → H2O(l) | ΔHf = −285.8 kJ/mol |
| (4) | C(s) + 2H2(g) → CH4(g) | ΔHf = ? kJ/mol |

Practice Problem 5: Use equations 1 and 2 below to calculate the ΔH values for equation 3. Is reaction 3 exothermic or endothermic?

|  |  |  |
| --- | --- | --- |
| (1) | ½ N2(g) + ½ O2(g) → NO(g) | ΔHf = 90.29 kJ/mol |
| (2) | ½ N2(g) + O2(g) → NO2(g) | ΔHf = 33.2 kJ/mol |
| (3) | NO(g) + ½O2(g) → NO2(g) | ΔH = ? kJ/mol |

e. In the above example equation 1 represents the formation of NO(g) from its elemental components. Equation 2 is the formation of NO2(g) from its elements.

**Heat of Formation:** represented by ΔHf is the energy released or absorbed (as heat) when one mole of a compound is formed by its *elements*.

Example: Mg(s) + Cl2(g) → MgCl2(s) ΔHf = - 641.5 kJ/mol

The table below lists ΔHf for a few common substances (also found on page 902).

|  |  |  |  |
| --- | --- | --- | --- |
| **Substance** |  | **Substance** |  |
| NH3(g) | −45.9 | HF(g) | −273.3 |
| NH4Cl(s) | −314.4 | H2O(g) | −241.82 |
| NH4F(s) | −125 | H2O(l) | −285.8 |
| NH4NO3(s) | −365.56 | H2O2(l) | −187.8 |
| Br2(l) | 0.00 | H2SO4(l) | −813.989 |
| CaCO3(s) | −1207.6 | FeO(s) | −825.5 |
| CaO(s) | −634.9 | Fe2O3(s) | −1118.4 |
| CH4(g) | −74.9 | MnO2(s) | −520.0 |
| C3H8(g) | −104.7 | N2O(g) | +82.1 |
| CO2(g) | −393.5 | O2(g) | 0.00 |
| F2(g) | 0.00 | Na2O(s) | −414.2 |
| H2(g) | 0.00 | Na2SO3(s) | −1101 |
| HBr(g) | −36.29 | SO2(g) | −296.8 |
| HCl(g) | −92.3 | SO3(g) | −395.7 |

Practice Problem 6: Calculate the heat of reaction value for the following reaction:

*CaCO3(s) → CaO(s) + CO2(g) ΔH=? kJ/mol*

Use heat of formation values. Is this reaction exothermic or endothermic?

f. The enthalpy of a final reaction can be rewritten using the following equation.

**ΔHreaction = (sum of ΔHf products) – (sum of ΔHf reactants)**

This equation states that the enthalpy change of a reaction is equal to the sum of the **enthalpies of formation** of the products minus the sum of the **enthalpies of formation** of the reactants. This allows Hess’s law to be extended to state that the enthalpy change of any reaction can be calculated by looking up the standard molar **enthalpy of formation, ,** of each substance involved. Look at example below:

Example: Calculate the enthalpy of reaction for the decomposition of hydrogen peroxide to water and oxygen gas according to the following equation.

2H2O2(l) → 2H2O(l) + O2(g)

|  |  |
| --- | --- |
| Items | Data |
| Δ*H* decomposition of H2O2(l) | ? kJ/mol |
|  | −187.8 kJ/mol\* |
|  | 0.00 kJ/mol\*\* |
|  | −285.8 kJ/mol\* |

\*from ΔHf Table on previous page \*\* any pure elemental substance has a of zero

**ΔHreaction = (sum of ΔHf products) – (sum of ΔHf reactants)**

ΔHreaction = [2(−285.8 kJ/mol) + 0.00 kJ/mol] − [2(−187.8 kJ/mol)] = −196.0 kJ/mol (exothermic reaction)

Practice Problem 7: Determine ΔH for each of the following reactions.

a. The following reaction is used to make CaO from limestone.

CaCO3(s) → CaO(s) + CO2(g) ans: 179.2 kJ/mol

b. The following reaction represents the oxidation of FeO to Fe2O3.

2FeO(s) +O2(g) → Fe2O3(s) ans: 533 kJ/mol

c. The following reaction of ammonia and hydrogen fluoride produces ammonium fluoride.

NH3(g) +HF(g) → NH4F(s) ans: 194 kJ/mol

**Example Problem: Determining Heats of Reactions**

1. Write the original equation. *CaCO3(s) → CaO(s) + CO2(g) ΔH=? kJ/mol*

2. Look at each reactant and each product and (if not already provided) write a formation equation for each. Look up correct *ΔHf* values. Multiply the ΔHf  value by the coefficient in front of that compound.

*2Ca + 2C + 3O2 → 2CaCO3(s) ΔHf = 2( - 1207.6 kJ/mol)*

*2Ca + O2 → 2CaO(s) ΔHf = 2( - 634.9 kJ/mol)*

*C + O2 → CO2(g) ΔHf = - 393.5 kJ/mol*

3. “Flip” the equations so that the reactants and products from the original equation are on the appropriate side of the arrow. If the equation was “flipped,” change the sign of the ΔHf value.

*2CaCO3(s) → 2Ca + 2C + 3O2 ΔHf = + 2415.2 kJ/mol*

*2Ca + O2 → 2CaO(s) ΔHf = - 1269.8 kJ/mol*

*C + O2 → CO2(g) ΔHf = - 393.5 kJ/mol*

4. If needed, multiply each equation by a whole number or a fraction to give the same coefficient as in the original equation. Multiply the ΔHf by the same whole number or fraction.

*½ (2CaCO3(s) → 2Ca + 2C + 3O2) ΔHf = ½ (+ 2415.2 kJ/mol )*

*½ (2Ca + O2 → 2CaO(s)) ΔHf = ½ ( - 1269.8 kJ/mol)*

*C + O2 → CO2(g) ΔHf = - 393.5 kJ/mol*

5. “Add” the reactions so that only the reactants and products that are left show the original equation.

*CaCO3(s) → ~~Ca~~ + ~~C~~ + ~~3/2 O~~~~2~~ ΔHf = + 1207.6 kJ/mol*

*~~Ca~~ + ~~1/2 O~~~~2~~ → CaO(s) ΔHf = - 634.9 kJ/mol*

*~~C~~ + ~~O~~~~2~~ → CO2(g) ΔHf = - 393.5 kJ/mol*

*CaCO3(s) → CaO(s) + CO2(g)* ***ΔH= + 179.2 kJ/mol***

Is reaction exothermic or endothermic?

**-ΔH = exothermic reaction** **+ΔH = endothermic reaction**

***If only ΔHf values are used then the following equation can also be used to solve this problem!***

**ΔHreaction = (sum of ΔHf products) – (sum of ΔHf reactants)**

**ΔHreaction = [(-634.9) + (-393.5)] – [-1207.6] = *+ 179.2 kJ/mol***