Heat of Reaction

The Heat of Reaction (also known and Enthalpy of Reaction) is the change in the enthalpy of a chemical reaction that occurs at a constant pressure. It is a thermodynamic unit of measurement useful for calculating the amount of energy per mole either released or produced in a reaction. Since enthalpy is derived from pressure, volume, and internal energy, all of which are state functions, enthalpy is also a state function.

Introduction

ΔH, or the change in enthalpy arose as a unit of measurement meant to calculate the change in energy of a system when it became too difficult to find the ΔU, or change in the internal energy of a system, by simultaneously measure the amount of heat and work exchanged. Given a *constant pressure*, the change in enthalpy can be measured as

$$\Delta H = q \tag{1}$$

See section on enthalpy for a more detailed explanation.

The notation ΔH^o or ΔH^o_{rxn} then arises to explain the precise temperature and pressure of the heat of reaction ΔH. The standard enthalpy of reaction is symbolized by ΔH^o or ΔH^o_{rxn} and can take on both positive and negative values. The units for ΔH^o are kiloJoules per mole, or kj/mol.

ΔH and ΔH^o_{rxn}

- Δ = represents the change in the enthalpy; ($\Delta H_{products}$ -$\Delta H_{reactants}$)
  - a positive value indicates the products have greater enthalpy, or that it is an endothermic reaction (heat is required)
  - a negative value indicates the reactants have greater enthalpy, or that it is an exothermic reaction (heat is produced)
- ^{o} = signifies that the reaction is a standard enthalpy change, and occurs at a preset pressure/temperature
- $_{rxn}$ = denotes that this change is the enthalpy of reaction

The Standard State: The standard state of a solid or liquid is the pure substance at a pressure of 1 bar (10^5 Pa) and at a relevant temperature.

The ΔH^o_{rxn} is the standard heat of reaction or standard enthalpy of a reaction, and like ΔH also measures the enthalpy of a reaction. However, ΔH^o_{rxn} takes place under "standard" conditions, meaning that the reaction takes place at 25º C and 1 atm. The benefit of a measuring ΔH under standard conditions lies in the ability to relate one value of ΔH^o to another, since they occur under the same conditions.

How to Calculate ΔH Experimentally

Enthalpy can be measured experimentally through the use of a calorimeter. A calorimeter is an isolated system which has a constant pressure, so $\Delta H = q = cp_{sp}$ x m x (ΔT)
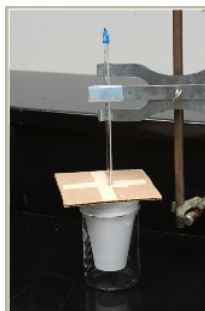
How to calculate ΔH Numerically

To calculate the standard enthalpy of reaction the standard enthalpy of formation must be utilized. Another, more detailed, form of the standard enthalpy of reaction includes the use of the standard enthalpy of formation ΔH^o_f:

$$\Delta H^{\ominus} = \sum \Delta v_p \Delta H_f^{\ominus} \, (products) - \sum \Delta v_r \Delta H_f^{\ominus} \, (reactants) \tag{2}$$

with

- v_p= stoichiometric coefficient of the product from the balanced reaction
- v_r= stoichiometric coefficient of the reactants from the balanced reaction
- $\Delta H°_f$= standard enthalpy of formation for the reactants or the products

Since enthalpy is a state function, the heat of reaction depends only on the final and initial states, not on the path that the reaction takes. For example, the reaction $A \rightarrow B$ goes through intermediate steps (i.e. $C \rightarrow D$), but A and B remain intact.

$$A \rightarrow C$$
$$C \rightarrow D$$
$$\underline{D \rightarrow B}$$
$$A \rightarrow B$$
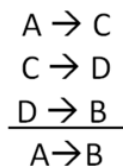
Therefore, one can measure the enthalpy of reaction as the sum of the ΔH of the three reactions by applying Hess' Law.

Additional Notes

Since the ΔHº represents the total energy exchange in the reaction this value can be either positive or negative.

- A positive ΔHº value represents an **addition** of energy from the reaction (and **from** the surroundings), resulting in an endothermic reaction.
- A negative value for ΔHº represents a **removal** of energy from the reaction (and **into** the surroundings) and so the reaction is exothermic.

Example 1: the combustion of acetylene

Calculate the enthalpy change for the combustion of acetylene (C_2H_2)

Solution

1) The first step is to make sure that the equation is balanced and correct. Remember, the combustion of a hydrocarbon requires oxygen and results in the production of carbon dioxide and water.

$$2\,C_2H_2(g) + 5\,O_2(g) \longrightarrow 4\,CO_2(g) + 2\,H_2O(g) \tag{3}$$
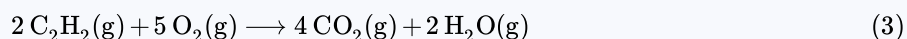
2) Next, locate a table of Standard Enthalpies of Formation to look up the values for the components of the reaction (Table 7.2, Petrucci Text)

3) First find the enthalpies of the products:

$$\Delta H°_f\ CO_2 = -393.5\ kJ/mole$$

Multiply this value by the stoichiometric coefficient, which in this case is equal to 4 mole.

$v_p\Delta H°_f\ CO_2 = 4\ mol\ (-393.5\ kJ/mole)$

$$= -1574\ kJ$$

$\Delta H°_f\ H_2O = -241.8\ kJ/mole$

The stoichiometric coefficient of this compound is equal to 2 mole. So,

$$v_p\Delta H°_f\ H_2O = 2\ mol\ (\ -241.8\ kJ/mole)$$

$= -483.6\ kJ$

Now add these two values in order to get the sum of the products

Sum of products (Σ $v_p\Delta H^o_f$(products)) = (-1574 kJ) + (-483.6 kJ) = -2057.6 kJ

Now, find the enthalpies of the reactants:

$$\Delta H^o_f\ C_2H_2 = +227\ kJ/mole$$

Multiply this value by the stoichiometric coefficient, which in this case is equal to 2 mole.

$$v_p\Delta H^o_f\ C_2H_2 = 2\ mol\ (+227\ kJ/mole)$$

= +454 kJ

$$\Delta H^o_f\ O_2 = 0.00\ kJ/mole$$

The stoichiometric coefficient of this compound is equal to 5 mole. So,

$$v_p\Delta H^o_f\ O_2 = 5\ mol\ (\ 0.00\ kJ/mole)$$

= 0.00 kJ

Add these two values in order to get the sum of the reactants

Sum of reactants (Δ $v_r\Delta H^o_f$(reactants)) = (+454 kJ) + (0.00 kJ) = +454 kJ

The sum of the reactants and products can now be inserted into the formula:

$\Delta H^o = \Delta$ $v_p\Delta H^o_f$(products) - ? $v_r\Delta H^o_f$(reactants)

= -2057.6 kJ - +454 kJ

= -2511.6 kJ

Practice Problems

1. Calculate ΔH if a piece of metal with a specific heat of .98 kJ·kg^{-1}·K^{-1} and a mass of 2 kg is heated from 22°C to 28°C.
2. If a calorimeter's ΔH is +2001 Joules, how much heat did the substance inside the cup lose?
3. Calculate the ΔH of the following reaction: $CO_{2\ (g)}$ + $H_2O_{\ (g)}$ --> $H_2CO_{3\ (g)}$ if the standard values of ΔH_f are as follows: $CO_{2\ (g)}$: -393.509 KJ /mol, $H_2O_{\ (g)}$: -241.83 KJ/mol, and $H_2CO_{3(g)}$: -275.2 KJ/mol.
4. Calculate ΔH if a piece of aluminum with a specific heat of .9 kJ·kg^{-1}·K^{-1} and a mass of 1.6 kg is heated from 286°K to 299°K.
5. If the calculated value of ΔH is positive, does that correspond to an endothermic reaction or an exothermic reaction?

Solutions

1. $\Delta H = q = cp_{sp}$ x m x (ΔT) = (.98) x (2) x (+6°) = 11.76 kJ
2. Since the heat gained by the calorimeter is equal to the heat lost by the system, then the substance inside must have lost the negative of +2001 J, which is -2001 J.
3. $\Delta H^{°} = \Sigma\Delta v_p\Delta H^{°}_f$(products) - $\Sigma\Delta$ $v_r\Delta H^{°}_f$(reactants) so this means that you add up the sum of the ΔH's of the products and subtract away the ΔH of the products: (-275.2kJ) - (-393.509kJ + -241.83kJ) = (-275.2) - (-635.339) = +360.139 kJ.
4. $\Delta H = q = cp_{sp}$ x m x (ΔT) = (.9) x (1.6) x (13) = 18.72 kJ
5. Endothermic, since a positive value indicates that the system GAINED heat.

References

1. Petrucci, et al. General Chemistry: Principles & Modern Applications. 9th ed. Upper Saddle River, New Jersey 2007.
2. Zumdahl, Steven S., and Susan A. Zumdahl. *Chemistry*. Boston: Houghton Mifflin Company, 2007.

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