CEN 207 Physical Chemistry

Text book:

Atkins' Physical Chemistry, Peter Atkins, Julio de Paula, James Keeler, 11th Edition, Oxford University Press.

Reference books

. Physical Chemistry, Robert J. Silbey, Robert A. Alberty, Moungi G. Bawendi

. Physical Chemistry, Ira N. Levine

THERMOCHEMISTRY

Thermochemistry: energy transferred during the course of chemical reaction.

If ΔU or ΔH for a reaction is known, it is possible to predict the heat the reaction can produce.

Exothermic (exenthalpic) process: $\Delta H<0$

Endothermic (endenthalpic) process: $\Delta H>0$

Standard enthalpy changes: under the a set of standard condition (1 bar, 298 K),

$H_2O(l) \rightarrow H_2O(g)$ $\Delta_{vap}H^{\ominus}$ (373 K): 40.66 kJ/mol

$H_2O(l) \rightarrow H_2O(g)$ $\Delta_{trs}H^{\ominus}$: 6.01 kJ/mol

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THERMOCHEMISTRY

Standard reaction enthalpy;

2A + B → 3C+D

$$\Delta_r H^\theta = \{3H_m^\theta(C) + H_m^\theta(D)\} - \{2H_m^\theta(A) + H_m^\theta(B)\}$$

$$\Delta H_r^\ominus = \Delta_r H^\theta = \sum_{products} \nu H_m^\theta - \sum_{reactants} \nu H_m^\theta$$ standard reaction enthalpy

Hess's Law:

Standard reaction enthalpies can be combined to obtain the value for another reaction. This application of the First Law is called Hess's Law.

The standard reaction enthalpy is the sum of the values for the individual reaction into which the overall reaction may be divided.

THERMOCHEMISTRY

Standard enthalpies of formation

$\Delta H_f^{\ominus}, \Delta_f H^{\ominus}$ $\quad\quad$ $\Delta_f H^{\ominus} = 0$ for elements,

For any reaction

$\Delta H_f^{\ominus} = \Delta_f H^{\theta} = \sum_{products} \nu H_f^{\theta} - \sum_{reactants} \nu H_f^{\theta}$ (practical implementation)

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THERMOCHEMISTRY

The temperature dependence of reaction enthalpies:

$$H(T_2) = H(T_1) + \int_{T_1}^{T_2} C_p dT$$

Enthalpy changes from T_1 to T_2,

The standard reaction enthalpy changes from

$$\Delta H_r^{\ominus}(T_2) = \Delta H_r^{\ominus}(T_1) + \int_{T_1}^{T_2} \Delta C_p^{\ominus} dT$$ Kirchhoff's Law

$$\Delta H_r^{\ominus}(T_2) = \Delta H_r^{\ominus}(T_1) + \Delta C_{p,r}^{\ominus}(T_2 - T_1)$$

$$\Delta C_{p,r}^{\ominus} = \sum_{products} \nu C_{p,m}^{\theta} - \sum_{reactants} \nu C_{p,m}^{\theta}$$

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