A First Course on Kinetics and Reaction Engineering
Unit 2. Reaction Thermochemistry

Definitions

standard heat of reaction - enthalpy change that occurs when stoichiometric amounts of reactants in their standard state are isothermally converted to stoichiometric amounts of products without any work being done

endothermic reaction - a reaction with a positive heat of reaction, that is, energy must be added when the reaction takes place

exothermic reaction - a reaction with a negative heat of reaction; energy is released when the reaction takes place

state function - a quantity, such as enthalpy, that is determined by the temperature pressure and composition (i. e. the state); when a system is transformed from one state to another, the change in the quantity is the same no matter what path the transformation followed

adiabatic process - a process wherein no heat or energy is added to or removed from the system

adiabatic temperature change/rise - the change in system temperature that occurs during an adiabatic reaction process

sensible heat - energy that is added/removed to/from a system and causes the temperature of the system to increase/decrease

latent heat - energy that is added/removed to/from a system and causes an isothermal phase change in the system

Nomenclature

$\Delta G_{f,i}^{0}\left(298 \text{ K}\right)$ standard Gibbs free energy change for the formation of species i at 298 K

$\Delta G_{j}^{0}\left(298 \text{ K}\right)$ standard Gibbs free energy change for reaction j at 298 K

$\Delta H_{c,i}(T)$ heat of combustion of species i at temperature T; a superscripted 0 indicates all species are in their standard states

$\Delta H_{f,i}(T)$ heat of formation of species i at temperature T; a superscripted 0 indicates all species are in their standard states

$\Delta H_{j}(T)$ heat of reaction j at temperature T; a superscripted 0 indicates all species are in their standard states

$\Delta H_{a \rightarrow b}$ sensible heat associated with a temperature change from a to b

$v_{i,j}$ stoichiometric coefficient of species i in reaction j; value is positive for products and negative for reactants

ξ_{j} extent of reaction j in a batch system (i. e. with units of moles)

$\hat{C}_{p,i}$ constant pressure specific molar heat capacity of species i

N_{ind} the number of mathematically independent chemical reactions taking place in a system

T temperature

n_i moles of species i; a superscripted 0 denotes an initial or starting value

Equations

$$\Delta H_j^0\left(298 \text{ K}\right) = \sum_{\substack{i= \text{ all} \\ \text{species}}} v_{i,j}\Delta H_{f,i}^0\left(298 \text{ K}\right) \tag{2.1}$$

$$\Delta H_j^0\left(298 \text{ K}\right) = \sum_{\substack{i= \text{ all} \\ \text{species}}} v_{i,j}\left(-\Delta H_{c,i}^0\left(298 \text{ K}\right)\right) \tag{2.2}$$

$$\Delta H_{T\rightarrow 298 \text{ K}}^0 = \sum_{\substack{i= \text{ all} \\ \text{reactants}}}\left(-v_{i,j}\int_T^{298K}\hat{C}_{p,i}\,dT\right) = \sum_{\substack{i= \text{ all} \\ \text{reactants}}}\left(v_{i,j}\int_{298K}^T\hat{C}_{p,i}\,dT\right) \tag{2.3}[1]$$

$$\Delta H_{298 \text{ K}\rightarrow T}^0 = \sum_{\substack{i= \text{ all} \\ \text{products}}}\left(v_{i,j}\int_{298K}^T\hat{C}_{p,i}\,dT\right) \tag{2.4}[1]$$

$$\Delta H_j^0\left(T\right) = \Delta H_j^0\left(298 \text{ K}\right) + \sum_{\substack{i= \text{ all} \\ \text{species}}}\left(v_{i,j}\int_{298K}^T\hat{C}_{p,i}\,dT\right) \tag{2.5}[1]$$

$$\sum_{j=1}^{N_{ind}}\xi_j\left(-\Delta H_j\left(T_1\right)\right) = \sum_{\substack{i=\text{all} \\ \text{species}}}\int_{T_1}^{T_2}\hat{C}_{p,i}\left(n_i^0+v_{i,j}\xi_j\right)dT \tag{2.6}[2]$$

$$\Delta G_j^0\left(298 \text{ K}\right) = \sum_{\substack{i=\text{all} \\ \text{species}}} v_{i,j}\Delta G_{f,i}^0\left(298 \text{ K}\right) \tag{2.7}$$

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[1] This equation is only valid if there is no phase change between 298 K and T.

[2] This equation is only valid for an adiabatic reaction where no phase change occurs between T_1 and T_2.