Thermodynamics

When heating a system, S increases where

$$\Delta S_u = \Delta S + \Delta S_s > 0 \tag{1}$$

and $\Delta \sum v > 0 \iff \Delta S > 0$. As well, $S \propto T \propto r \propto V \propto n \propto P^{-1}$ where n is the moles the side to which equilibrium moves to has.

The Born Haber cycle is used to find H_f of an ionic compound MX,

$$\Delta H_f = \sum H \qquad H_B = \tfrac{1}{2}B \tag{2}$$

where the sub-reactions are given by

$$\begin{aligned} \Delta H_s: &\quad M(s) \to M(g) \\ IE: &\quad M(g) \to M^+ + e^- \\ \tfrac{1}{2}B: &\quad \tfrac{1}{2}X_2 \to X \\ -EA: &\quad X + e^- \to X^- \\ -\Delta H_l: &\quad M^+ + X^- \to MX \end{aligned} \tag{3}$$

The change in $X : \{S, G, \Delta H_f\}$ is

$$\Delta X^\ominus = \Delta \sum v X^\ominus \tag{4}$$

If $G < 0$ the reaction is spontaneous.

Equilibrium

The equilibrium constant is given by

$$K_c \sim K_p = K_c R T^{\Delta v_h} \tag{5}$$

where K_p is for gaseous reactions. Reactions are homogeneous iff it is the same phase.

To calculate the eq. concentrations, construct an ICE table where

$$[A_i]_{eq} = [A_i] \mp ax \tag{6}$$

More reactants are formed in a reaction where

$$[A] \uparrow \iff [B] \downarrow \iff Q > K \tag{7}$$

Exothermic reactions produce heat such that if temperature increases as well, more reactants are formed.

For a reaction $A(s) \leftrightharpoons bB(aq)$, the constant

$$K_s p = [B]^b \iff x = (K_{sp}/\Pi b^b)^{1/\Sigma b} \tag{8}$$

Materials Science

The density of a unit cell is given by

$$\rho = \frac{nM}{a^3 N_a} \qquad a = \left\{2r,\ 4r/\sqrt{3},\ 2\sqrt{2}r\right\} \tag{9}$$

for sc, bcc, and fcc respectively. The packing efficiency is given by nV_{sph}/a^3.

In semiconductors, temperature and impurities are proportional to conductivity, and opposite for conductors.

Thermoplastic polymers melt and deform upon heating. The DP is $\overline{M}/M_m$ and the average molecular weight is

$$\overline{M}_n = \frac{\Sigma MN}{\Sigma N} \qquad \overline{M}_w = \frac{\Sigma M^2 N}{\Sigma MN} \tag{10}$$

where $n_{\text{chains}} = mN_a/\overline{M}$. Polymers are linear, branched, and crosslinked.

The former two are connected by non-bonded interactions and can be easily recycled, and the latter by covalent bonds.

Linear polymers form crystals more easily and thus become liquid when heated.

Miscellaneous

A ketone is –C(=O)–; amides, carboxylics, aldehydes, and esters are KN–, KOH, KH, and KO–.

For stoichiometric problems, use

$$n_1/v_1 = n_2/v_2 \tag{11}$$

where $n = m/M = CV$. For an equilibrium reaction, the constant is K_c and only includes gaseous or aqueous compounds.

The partial pressure of a gas is

$$P_i = X_i P \qquad X_i = n_i/\sum n \qquad P = \sum P_i \tag{12}$$

For a reactant A dissociated δ%, then

$$P_A = (1-\delta)x \qquad P_B = (v_b \delta/v)ax \tag{13}$$

where the mole fraction is

$$x_i = m_i M/mM_i = n_i/n \tag{14}$$

The force in liquids is proportional to BP, viscosity, number of OH^- ions, H, and inversely proportional to P and T.