## 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,

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

where the sub-reactions are given by

$$\Delta H_s: \qquad M(s) \to M(g)$$

$$IE: \qquad M(g) \to M^+ + e^-$$

$$\frac{1}{2}B: \qquad \frac{1}{2}X_2 \to X \qquad (3)$$

$$-EA: \qquad X + e^- \to X^-$$

$$-\Delta H_t: \qquad M^+ + X^- \to MX$$

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

$$K_c \sim K_v = K_c R T^{\Delta v_g} \tag{5}$$

where  $K_p$  is for gaseous reactions. Reactions are homogeneous iff it is the same phase. More reactants are formed in a reaction where

$$[A] \uparrow \iff [B] \downarrow \iff Q > K \tag{6}$$

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

$$K_{sp} = [B]^b \iff x = (K_{sp}/\Pi b^b)^{1/\Sigma b}$$
 (7)

## Materials Science

The density of a unit cell is given by

$$\rho = \frac{m}{a^3 N_a} \qquad a = \left\{ 2r, \, 4r/\sqrt{3}, \, 2\sqrt{2}r \right\} \tag{8}$$

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

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

$$\overline{M}_n = \frac{\Sigma MN}{\Sigma N} \qquad \overline{M}_w = \frac{\Sigma M^2 N}{\Sigma MN}$$
 (9)

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

$$n_1/v_1 = n_2/v_2 \tag{10}$$

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

$$P_i = X_i P$$
  $X_i = n_i / \sum n$   $P = \sum P_i$  (11)

For a reactant A dissociated  $\delta$ %, then

$$P_A = (1 - \delta)x \qquad P_B = (v_b \delta / v) ax \tag{12}$$

where the mole fraction is  $x_i = n_i/n$ . The force in liquids is proportional to BP, viscosity, number of OH<sup>-</sup>ions, H, and inversely proportional to P and T.

In calorimetry, the heats are related via

$$-m_1 C_1 \Delta T_{f1} = m_2 C_2 \Delta T_{f2} \, \text{J/g} \tag{13}$$