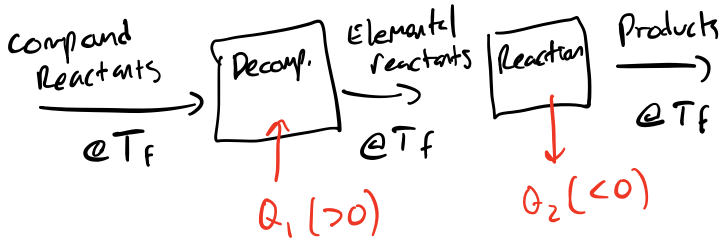
Recap

Heat of formation = Enthalpy of formation = Heat of reaction

$\bar{h}_f^o = Q_f$



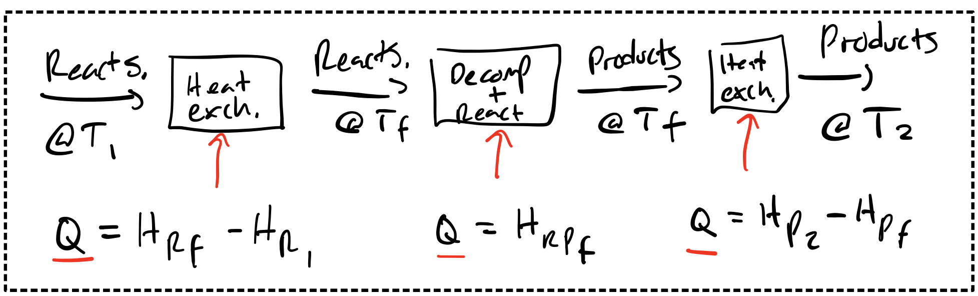
$$Q_1 = -\sum_i (n_i Q f_i)_{Reactants} \quad (>0) \text{ supply heat}$$

$$Q_2 = \sum_j (n_j Q f_j)_{products} \quad (<0) \text{ release (take away) heat}$$

i, j indices to count thru all reactants & products

$$Q_1 + Q_2 \equiv H_{RP_f}$$

In general, reactants & products do not enter/exit @ T_f → Redraw sketch



adiabatic container, ⇒ $Q_{Net} = 0$

$$H_{R_f} - H_{R_1} = \sum_i \left[n_i \overline{c_{p_i}} (T_f - T_1) \right]_{\text{Reactants}}$$

$$H_{RP_f} = \sum_j (n_j Q_{f_j})_{\text{products}} - \sum_i (n_i Q_{f_i})_{\text{Reactants}}$$

$$H_{P_2} - H_{P_f} = \sum_j \left[n_j \overline{c_{p_j}} (T_2 - T_f) \right]_{\text{products}}$$

$$Q_{net} = 0$$

$$\sum_j \left[n_j \overline{c_{p_j}} (T_2 - T_f) \right]_{\text{products}} = \sum_i \left[n_i \overline{c_{p_i}} (T_f - T_1) \right]_{\text{Reactants}}$$

$$+ \sum_i (n_i Q_{f_i})_{\text{Reactants}} - \sum_j (n_j Q_{f_j})_{\text{Products}}$$

$T_2 \equiv$ adiabatic flame temperature

T_f known

T_1 " (in this class, usually $T_1 = T_f$)

$\overline{c_{p_{i,j}}}$ known, $Q_{f_{i,j}}$ known, n_i, known

If n_j known (product composition),

can calculate T_2

Composition of Products

Problem: compos. of prod. (n_j) depends upon T

& T_2 " " n_j

e.g. w/in certain temp. range, water resulting from

$H_2 + \frac{1}{2} O_2$ React. dissociates into various components.

$$a H_2 + b O_2 \rightarrow c H_2O + d O_2 + e H_2 + f O + g H + h OH \quad (1)$$

Book uses $A H_2 + B O_2 \rightarrow n_{H_2O} H_2O \ldots$

a, b known

c, d, e, f, g, h unknown

to determine ↑, need 6 eqs

- start w/ mass balance

1 eqn for H atoms,

" " " O "

→ need 4 more - they come from chemical equilibrium

In (1), chem. equil. occurs entirely on RHS

In general, @ equil.

$$\underbrace{\alpha}_{\#\text{ of moles}} \underbrace{A}_{\text{species}} + \beta B \rightleftharpoons \mu M + \nu N \quad \Big\} \text{ on RHS}$$

For the A, B, M, N species,

Partial pressures are P_A, P_B, P_M, P_N

AND $\frac{P_i}{P_m} = \chi$ (mole frac)

From chemistry:

$$\frac{P_M^{\mu} \, P_N^{\nu}}{P_A^{\alpha} \, P_B^{\beta}} = K_p(T) \quad \text{const. of equilibrium}$$

There is also an equil. const. based on mole fractions themselves

$$K_n(T) \equiv \frac{\chi_M^{\mu} \chi_N^{\nu}}{\chi_A^{\alpha} \chi_B^{\beta}} = \frac{\left(\frac{P_M}{P_m}\right)^{\mu} \left(\frac{P_N}{P_m}\right)^{\nu}}{\left(\frac{P_A}{P_m}\right)^{\alpha} \left(\frac{P_B}{P_m}\right)^{\beta}} = P_m^{\alpha+\beta-\mu-\nu} K_p(T)$$

Typically, $K_p(T)$ $\begin{cases} \text{tabulated} \\ \text{plotted} \\ \text{analytical expr.} \end{cases}$

Ex. 1 mol H_2O heated to 3600 K @ 1atm

A fraction x of that mole dissociates into H_2 & O_2 $\quad K_p$ available in fig. 2.12

Task: determine x

@ equil.

$$1\, H_2O \rightleftharpoons \underbrace{(1-x)\, H_2O}_{\text{undissoc.}} + \underbrace{x\, H_2 + \tfrac{x}{2} O_2}_{\text{from dissoc.}}$$

mole count on RHS:

$(1-x)$ moles undissoc. H_2O

x 〃 H_2

$\frac{x}{2}$ 〃 O_2

$1+\frac{x}{2}$

$$x_{H_2O} = \frac{1-x}{1+\frac{x}{2}}$$

$$x_{H_2} = \frac{x}{1+\frac{x}{2}}$$

$$x_{O_2} = \frac{x/2}{1+x/2}$$

Dissoc. Equil. is

$$x\,H_2O \rightleftharpoons x\,H_2 + \frac{x}{2}O_2$$

$$H_2O \rightleftharpoons H_2 + \frac{1}{2}O_2$$

$$\Rightarrow K_p = \frac{(P_{H_2})^1 (P_{O_2})^{1/2}}{(P_{H_2O})^1}$$

And

$$K_N = \frac{x_{H_2}(x_{O_2})^{1/2}}{x_{H_2O}} = \frac{\left(\frac{x}{1+\frac{x}{2}}\right)\left(\frac{x/2}{1+\frac{x}{2}}\right)^{1/2}}{\frac{1-x}{1+x/2}} = \frac{x^{3/2}}{(1-x)\sqrt{2+x}}$$