6. Routes for calculating the free energy change in chemical reactions

A. From $\Delta G = \Delta H - T\Delta S$:

Example 17.9: **Consider thee reaction:**

$$2SO_2\,(g) + O_2\,(g) \longrightarrow 2SO_3\,(g)$$

Calculate $\Delta H°$, $\Delta S°$ and $\Delta G°$:

Substance	ΔH_f° (kJ/mol)	S° (J/mol · K)
SO_2 (g)	–297	248
SO_3 (g)	–396	257
O_2 (g)	0	205

- **Calculation of $\Delta H°$:**

$$\Delta H^\circ_{Rxn} = \sum_p n_p \Delta H_f^\circ(\text{products}) - \sum_r n_r \Delta H_f^\circ(\text{reactants})$$
$$= 2\Delta H_f^\circ(SO_3) - 2\Delta H_f^\circ(SO_2) - \Delta H_f^\circ(O_2)$$
$$= 2(-396) - 2(-297) - 0 \quad = -198\ \text{kJ}$$

- **Calculation of $\Delta S°$:**

$$\Delta S^\circ_{Rxn} = \sum_p n_p S^\circ(\text{products}) - \sum_r n_r S^\circ(\text{reactants})$$
$$= 2S^\circ(SO_3) - 2S^\circ(SO_2) - S^\circ(O_2)$$
$$= 2(257) - 2(248) - 205 \quad = -187\ \text{J/K}$$

• **Calculation of $\Delta G°$:**

$$\Delta G° = \Delta H° - T\Delta S° = -198 - (298)(-187\times10^{-3})$$

$$= -142 \text{ kJ}$$

B. From Free energies of formation ($\Delta G°_f$):

Example 17.11: Methanol is a high-octane fuel used in high-performance racing engines. Calculate $\Delta G°$ for the reaction:

$$2CH_3OH\,(g) + 3O_2\,(g) \longrightarrow 2CO_2\,(g) + 4H_2O\,(g)$$

Substance	ΔG_f° (kJ/mol)
CH_2OH (g)	–163
O_2 (g)	0
CO_2 (g)	–394
H_2O (g)	–229

$$\Delta G^\circ_{Rxn} = \sum_p n_p \Delta G^\circ_f(\text{products}) - \sum_r n_r \Delta G^\circ_f(\text{reactants})$$

$$= 2\Delta G^\circ_f(CO_2) + 4\Delta G^\circ_f(H_2O) - 3\Delta G^\circ_f(O_2) - 2\Delta G^\circ_f(CH_3OH)$$

$$= 2(-394) + 4(-229) - 2(-163) - 3\times0 = -1378 \text{ kJ}$$

C. From Hess's Law:

Given:

$2CH_4\,(g) + 3O_2\,(g) \longrightarrow 2CO\,(g) + 4H_2O\,(g)$

$\Delta G° = -1088$ kJ

$CH_4\,(g) + 2O_2\,(g) \longrightarrow CO_2\,(g) + 2H_2O\,(g)$

$\Delta G° = -801$ kJ

Calculate $\Delta G°$ for the reaction:

$$2CO\,(g) + O_2\,(g) \longrightarrow 2CO_2\,(g)$$

Invert Reaction (1):

$2CO\,(g) + 4H_2O\,(g) \longrightarrow 2CH_4\,(g) + 3O_2\,(g)$ $+1088$ kJ

Multiply Reaction (2) by 2:

$2CH_4\,(g) + 4O_2\,(g) \longrightarrow 2CO_2\,(g) + 4H_2O\,(g)$

-2×801 kJ

$$2CO\,(g) + O_2\,(g) \longrightarrow 2CO_2\,(g)$$

$\Delta G° = -514$ kJ

D. From the Equilibrium Constant *K* !

$$\Delta G° = -RT \ln K$$