

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

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

Example 17.9: Consider the reaction:



Calculate  $\Delta H^\circ$ ,  $\Delta S^\circ$  and  $\Delta G^\circ$ :

Substance	$\Delta H_f^\circ$ (kJ/mol)	$S^\circ$ (J/mol · K)
SO <sub>2</sub> (g)	-297	248
SO <sub>3</sub> (g)	-396	257
O <sub>2</sub> (g)	0	205

### • Calculation of $\Delta H^\circ$ :

$$\begin{aligned}\Delta H_{Rxn}^\circ &= \sum_p n_p \Delta H_f^\circ(\text{products}) - \sum_r n_r \Delta H_f^\circ(\text{reactants}) \\ &= 2\Delta H_f^\circ(\text{SO}_3) - 2\Delta H_f^\circ(\text{SO}_2) - \Delta H_f^\circ(\text{O}_2) \\ &= 2(-396) - 2(-297) - 0 = \mathbf{-198 \text{ kJ}}\end{aligned}$$

### • Calculation of $\Delta S^\circ$ :

$$\begin{aligned}\Delta S_{Rxn}^\circ &= \sum_p n_p S^\circ(\text{products}) - \sum_r n_r S^\circ(\text{reactants}) \\ &= 2S^\circ(\text{SO}_3) - 2S^\circ(\text{SO}_2) - S^\circ(\text{O}_2) \\ &= 2(257) - 2(248) - 205 = \mathbf{-187 \text{ J/K}}\end{aligned}$$

• Calculation of  $\Delta G^\circ$ :

$$\Delta G^\circ = \Delta H^\circ - T \Delta S^\circ = -198 - (298) (-187 \times 10^{-3})$$
$$= -142 \text{ kJ}$$

**B. From Free energies of formation ( $\Delta G_f^\circ$ ):**

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

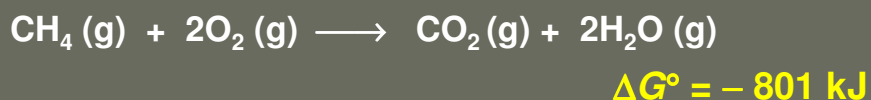


Substance	$\Delta G_f^\circ$ (kJ/mol)
CH <sub>3</sub> OH (g)	-163
O <sub>2</sub> (g)	0
CO <sub>2</sub> (g)	-394
H <sub>2</sub> O (g)	-229

$$\Delta G_{\text{Rxn}}^\circ = \sum_p n_p \Delta G_f^\circ (\text{products}) - \sum_r n_r \Delta G_f^\circ (\text{reactants})$$
$$= 2\Delta G_f^\circ (\text{CO}_2) + 4\Delta G_f^\circ (\text{H}_2\text{O}) - 3\Delta G_f^\circ (\text{O}_2)$$
$$- 2\Delta G_f^\circ (\text{CH}_3\text{OH})$$
$$= 2(-394) + 4(-229) - 2(-163) - 3 \times 0 = -1378 \text{ kJ}$$

C. From Hess's Law:

Given:



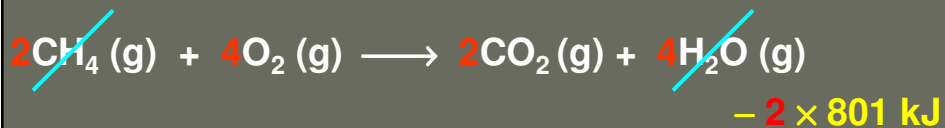
Calculate  $\Delta G^\circ$  for the reaction:



**Invert Reaction (1):**



**Multiply Reaction (2) by 2:**



$$\Delta G^\circ = -514 \text{ kJ}$$

D. From the Equilibrium Constant  $K$ !

$$\Delta G^\circ = -RT \ln K$$