

19.2 Calculating Entropy Change

Entropy Change in the Surroundings

Consider the reaction $\text{N}_2(\text{g}) + 2\text{H}_2\text{O}(\text{l}) = 2\text{NO}(\text{g}) + 2\text{H}_2(\text{g})$
for which $\Delta H^\circ = 752.2 \text{ kJ}$ and $\Delta S^\circ = 351.6 \text{ J/K}$ at 298.15 K

- At 298.15 K is this reaction product or reactant favored?
- Is the answer to a) entropy or enthalpy driven?

$$\Delta S^\circ_{\text{UNIV}} = \Delta S^\circ_{\text{SYS}} + \Delta S^\circ_{\text{SURR}}$$

$$\Delta S^\circ_{\text{SYS}} = \Delta S^\circ_{\text{RXN}} = 351.6 \text{ J/K}$$

$$\begin{aligned}\Delta S^\circ_{\text{SURR}} &= -\frac{\Delta H^\circ_{\text{RXN}}}{T} \\ &= -\frac{752,200 \text{ J}}{298.15 \text{ K}} = -2522.8 \text{ J/K}\end{aligned}$$

$$\begin{aligned}\Delta S^\circ_{\text{UNIV}} &= 351.6 - 2522.8 \\ &= -2171.2 \text{ J/K}\end{aligned}$$

a) $\Delta S^\circ_{\text{UNIV}} < 0$
Nonspontaneous, reactant favored.

b) $\Delta S^\circ_{\text{SYS}} > 0$
 $\Delta S^\circ_{\text{SURR}} < 0$... determined by ΔH°
Thus $\Delta S^\circ_{\text{UNIV}} < 0$ is enthalpy driven.

NOTE: To reduce the impact of $\Delta S^\circ_{\text{SURR}}$, then move away from standard temperature condition. Substantially increasing T would increase the effect of $\Delta S^\circ_{\text{SURR}}$ and one could find a T in which $\Delta S^\circ_{\text{SURR}}$ becomes > 0 .
This leads us to GIBBS FREE ENERGY.

19.3 Gibbs Free Energy

Gibbs Free Energy and Spontaneity

$$G = H - TS \quad G = \text{Gibbs Free Energy}$$
$$\Delta G = \Delta H - T\Delta S$$

$$\Delta S_{\text{univ}} = \Delta S_{\text{sys}} - \frac{\Delta H_{\text{sys}}}{T} > 0 \quad \text{for a spontaneous reaction.}$$

$$\Delta S_{\text{sys}} - \frac{\Delta H_{\text{sys}}}{T} > 0$$
$$T\Delta S_{\text{sys}} - \Delta H_{\text{sys}} > 0$$
$$\underbrace{-T\Delta S_{\text{sys}} + \Delta H_{\text{sys}}}_{\Delta G_{\text{sys}}} < 0$$

$$\Delta G_{\text{sys}} < 0 \quad \text{for a spontaneous reaction.}$$

Gibbs Free Energy = the maximum work we can get from a reaction.

$\Delta G < 0$: spontaneous in the forward direction.

$\Delta G > 0$: nonspontaneous in the forward direction ... conversely spontaneous in the reverse direction.

$\Delta G = 0$: at equilibrium

19.3 Gibbs Free Energy

Standard Gibbs Free Energy

Two main methods to determine $\Delta G_{\text{RXN}}^{\circ}$

1.
$$\Delta G_{\text{RXN}}^{\circ} = \Delta H_{\text{RXN}}^{\circ} - T\Delta S_{\text{RXN}}^{\circ}$$

2.
$$\Delta G_{\text{RXN}}^{\circ} = \sum \Delta G_f^{\circ} (\text{products}) - \sum \Delta G_f^{\circ} (\text{reactants})$$

Similar to ΔH_f° are tabulated for a host of molecules.
Just like ΔH_f° for an element in its standard stat,
the ΔG_f° for an element in its standard state is zero.

