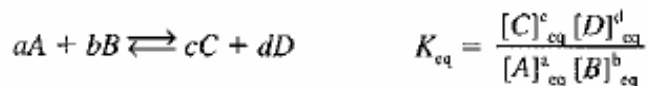


Základní vztahy k procvičení

$$\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ$$

$$\Delta G^\circ_{\text{reaction}} = \sum \text{coeff}_p \Delta G^\circ_f(\text{products}) - \sum \text{coeff}_r \Delta G^\circ_f(\text{reactants})$$



$$\Delta G = \Delta G^\circ + RT \ln Q$$

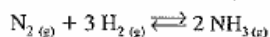
$$0 = \Delta G^\circ + RT \ln K_{\text{eq}} \quad \Delta G^\circ = -RT \ln K_{\text{eq}}$$

Kniha:

J. Olmsted III, G. M. Williams: Chemistry – The Molecular Science, Moshby – Year Book, Inc., 1994

EXAMPLE PROBLEM 15-9 THERMODYNAMICS AND K_{eq}

Using standard thermodynamic data, find the value of K_{eq} at 298 K for the Haber reaction:



METHOD: Equation 15-5 provides the link between thermodynamic data and K_{eq} . We must calculate $\Delta G^\circ_{\text{rxn}}$ from tabulated standard free energies of formation.

$$\Delta G^\circ_{\text{rxn}} = \sum (\text{coeff}) \Delta G^\circ_f(\text{products}) - \sum (\text{coeff}) \Delta G^\circ_f(\text{reactants})$$

Appendix E contains the appropriate values:

$$\Delta G^\circ_f \text{ (kJ/mol): } \text{N}_2(g), 0; \text{H}_2(g), 0; \text{NH}_3(g), -16.4 \text{ kJ/mol}$$

$$\Delta G^\circ = (2 \text{ mol NH}_3)(-16.4 \text{ kJ/mol NH}_3) - 3(0) - 1(0) = -32.8 \text{ kJ}$$

To determine the equilibrium constant, Equation 15-5 must be rearranged to isolate $\ln K_{\text{eq}}$.

$$\ln K_{\text{eq}} = -\frac{\Delta G^\circ}{RT} = \frac{-(-32.8 \text{ kJ})(10^3 \text{ J/kJ})}{(8.314 \text{ J/K})(298 \text{ K})} = 13.24$$

$$K_{\text{eq}} = e^{13.4} = 5.6 \times 10^5 \text{ atm}^{-2}$$

The exponential gives a dimensionless number, since e^x is always a pure number. However, we assign units to K_{eq} as required by the concentration quotient. Remember that the superscript "o" in ΔG° refers to standard conditions that include concentrations of 1 M for solutes and 1 atm partial pressure for gases.

Remember that ΔG°_f for any element in its standard state is zero.

SAMPLE PROBLEM 15-10 K_{eq} AND TEMPERATURE

Use tabulated thermodynamic data to estimate K_{eq} for the Haber reaction at 500 °C.

METHOD: Values for ΔH° and ΔS° can be calculated using tabulated thermodynamic values. Then Equation 15-6 can be applied to determine the value of the equilibrium constant at 500 °C. First, we need ΔH°_{rxn} and ΔS°_{rxn} :

$$\Delta H^\circ_{rxn} = \sum (\text{coeff}) \Delta H^\circ_f (\text{products}) - \sum (\text{coeff}) \Delta H^\circ_f (\text{reactants})$$

$$\Delta S^\circ_{rxn} = \sum (\text{coeff}) S^\circ (\text{products}) - \sum (\text{coeff}) S^\circ (\text{reactants})$$

Appendix E contains the appropriate values:

ΔH°_f (kJ/mol)	$N_2(g)$: 0	$H_2(g)$: 0	$NH_3(g)$: -46
S° (J/mol K)	$N_2(g)$: 191.6	$H_2(g)$: 130.7	$NH_3(g)$: 192.45

$$\Delta H^\circ_{rxn} = (2)(-46 \text{ kJ/mol}) - 3(0) - 0 = -92 \text{ kJ/mol}$$

$$\Delta S^\circ_{rxn} = (2)(192.45 \text{ J/mol K}) - (3)(130.7 \text{ J/mol K}) - 191.6 \text{ J/mol K}$$

$$\Delta S^\circ_{rxn} = -198.8 \text{ J/mol K}$$

Now calculate K_{eq} at 500 °C using Equation 15-6:

$$\ln K_{eq} = \frac{\Delta H^\circ}{RT} + \frac{\Delta S^\circ}{R}$$

$$\ln K_{eq} = -\frac{(-92 \text{ kJ/mol})(10^3 \text{ J/kJ})}{(8.314 \text{ J/mol K})(500 + 273 \text{ K})} + \frac{(-198.8 \text{ J/mol K})}{(8.314 \text{ J/mol K})}$$

$$\ln K_{eq} = 14.3 - 23.9 = -9.6$$

Taking the anti/ \ln , or e^x , of -9.6 gives the estimated equilibrium constant at 500 °C:

$$K_{eq} = 6.7 \times 10^{-5} \text{ atm}^{-2}$$