

Q. In the gas-phase reaction $2A + B \rightleftharpoons 3C + 4D$, it was found, when 1.0 mole A, 2 mole B, 1 mole D were mixed and allowed to come to equilibrium at 25°C, the resulting contained 0.90 mole of C at a total pressure of 1 bar. Calculate 1) the mole fraction of each species at equm. 2) K_p

⇒ The given reaction is $2A + B \rightleftharpoons 3C + 4D$. Initial mo of moles are $n_A^0 = 1$, $n_B^0 = 2$, $n_D^0 = 1$. Let at equm x mole B reacts ^{then} $2x$ mole A react and $3x$ mole C and $4x$ mole D are produced. So at equilibrium number of mole of C = $3x = 0.90$. So $x = 0.3$

at equilibrium

$$n_A = n_A^0 - 2x = 1 - 2 \times 0.3 = 0.4$$

$$n_B = n_B^0 - x = 2 - 0.3 = 1.7$$

$$n_C = 3x = 0.90$$

$$n_D = n_D^0 + 4x = 1 + 4 \times 0.3 = 2.2$$

Mole fraction

$$x_A = \frac{n_A}{\sum n} = \frac{0.4}{5.2} = 0.07$$

$$x_B = \frac{n_B}{\sum n} = \frac{1.7}{5.2} = 0.32$$

$$x_C = \frac{n_C}{\sum n} = \frac{0.9}{5.2} = 0.17$$

$$x_D = \frac{n_D}{\sum n} = \frac{2.2}{5.2} = 0.423$$

$$\text{Equm. constant } K_p = \frac{n_C^3 \cdot n_D^4}{n_A^2 \cdot n_B} \cdot \left(\frac{P}{\sum n} \right)^{\Delta n}$$

$$\Delta n = (3+4) - (2+1) = 4$$

$$K_p = \frac{(0.9)^3 \cdot (2.2)^4}{(0.4)^2 \times 1.7} \left(\frac{1}{5.2} \right)^4 = \frac{0.729 \times 23.4}{0.16 \times 1.7} = 0.085$$

$$\Delta G^\circ = -RT \ln K_p = 8.314 \times 298 \ln 0.085 = 6084.26 \text{ Joule.}$$

Q. Ferrrous sulphate undergoes decomposition as $2\text{FeSO}_4(\text{s}) = \text{Fe}_2\text{O}_3(\text{s}) + \text{SO}_2(\text{g}) + \text{SO}_3(\text{g})$ at 929K total gas pressure = 0.9 atm. With both solid presents. Calculate 1) K_p 2) Equilibrium total pressure, If excess FeSO_4 is placed with initial SO_2 pressure of 0.6 atm.

$$\Rightarrow K_p = P_{\text{SO}_2} \cdot P_{\text{SO}_3}, \text{ Initially } P_{\text{SO}_2} = P_{\text{SO}_3}$$

$$P_{\text{SO}_2} + P_{\text{SO}_3} = 0.9 \text{ atm}$$

$$P_{\text{SO}_2} = P_{\text{SO}_3} = 0.45 \text{ atm}$$

$$K_p = (0.45)^2 = 0.2025$$

When initial pressure of $\text{SO}_2 = 0.6 \text{ atm}$

$$\text{Let } P_{\text{SO}_3} = x$$

$$\text{So } P_{\text{SO}_2} = (0.6 + x)$$

$$\text{Hence, } (0.6 + x)x = 0.2025$$

$$x = 0.24$$

$$\text{Total pressure} = 0.6 + x + x = 1.08 \text{ atm}$$

Q. A mixture is composed of A and B in the molar ratio 1 : 0.3. For a change of -10 J mole^{-1} in the chemical potential of A what would be corresponding change in chem. pot. of B.

$\Rightarrow$ From Gibbs - Duhem equation

$$\sum n_i d\mu_i = 0$$

$$\text{So, } n_A \cdot d\mu_A + n_B d\mu_B = 0$$

In the given problem if $n_A = 1$. $n_B = 0.3$

$$\text{Also, } d\mu_A = -10 \text{ J} \cdot \text{mole}^{-1} \quad d\mu_B = ?$$

$$1 \times (-10) + 0.3 d\mu_B = 0$$

$$\text{on, } d\mu_B = \frac{10}{0.3} = 33.3 \text{ J} \cdot \text{mole}^{-1}$$

Q. Calculate the free energy change accompanying the compression of 1 mole of a gas at 57°C from 25 to 200 atm. The fugacities of the gas at 57°C may be taken as 23 and 91 atm, respectively at pressure 25 and 200 atm.

$$\begin{aligned} \Rightarrow \Delta G &= nRT \ln \frac{P_2}{P_1} = 1 \text{ mole} \times 8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mole}^{-1} \times 330 \text{ K} \\ &\quad \ln \frac{200 \text{ atm}}{25 \text{ atm}} \\ &= 5702.8 \text{ J} \end{aligned}$$

$$\begin{aligned} \Delta G &= nRT \ln \frac{f_2}{f_1} = 1 \text{ mole} \times 8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mole}^{-1} \times 330 \text{ K} \ln \frac{91 \text{ atm}}{23 \text{ atm}} \\ &= 3730.0 \text{ J} \end{aligned}$$

Q. The activity of 2.5 mole of a substance change from 0.05 to 0.35. What be the change in its free energy at 27°C.

$$\Rightarrow \Delta G = RT \ln \frac{a_2}{a_1}$$

$$\begin{aligned}\text{For } n \text{ mole, } \Delta G &= nRT \ln \frac{a_2}{a_1} \\ &= 2.5 \text{ mole} \times 8.314 \text{ J K}^{-1} \cdot \text{mol}^{-1} \cdot (300\text{K}) \ln \frac{0.35}{0.05} \\ &= 12133.6 \text{ J}\end{aligned}$$

Q. 4.0 mole N_2 at 1 atm and 300K and 2 mole of H_2 at 2 atm and 300K are mixed in a container. Assuming the gases to behave ideally calculate the change in free energy ΔG_{mix} and enthalpy ΔH_{mix} due to mixing.

$\Rightarrow$ For isothermal mixing

$$\Delta G_{\text{mix}} = nRT \sum x_i \ln x_i$$

$$n = 4 + 2 = 6 \quad T = 300 \quad x_{\text{N}_2} = \frac{4}{6} = \frac{2}{3}, \quad x_{\text{H}_2} = \frac{1}{3}$$

$$\begin{aligned}\Delta G_{\text{mix}} &= 6 \times 8.313 \times 300 \left[\frac{2}{3} \ln \frac{2}{3} + \frac{1}{3} \ln \frac{1}{3} \right] \text{ Jolue} \\ &= -9524.4 \text{ Jolue}\end{aligned}$$

For isothermal mixing $\Delta H_{\text{mix}} = 0$ (for ideal gas)