B10704007 [illegible]

Thermodynamics of Materials II Homework#4

$1\ atm = 760\ mmHg = 1.01 \times 10^5\ N\ m^{-2}, R = 8.314\ J\ mol\ K^{-1}$

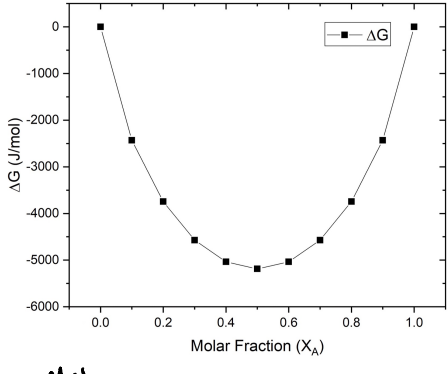
1 The A-B solution forms an ideal solution at 900 K. Answer the below questions.

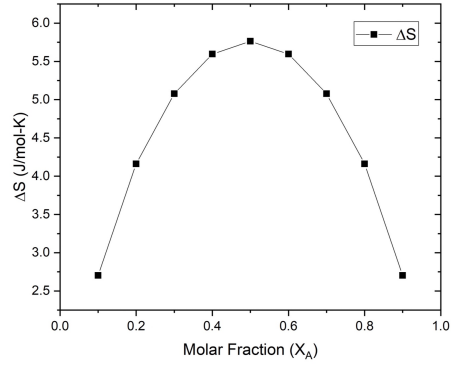
1.1 Plot $\Delta G^{M,id}\ vs.\ X_A$ and $\Delta S^{M,id}\ vs.\ X_A$.

1.2 Calculate $\Delta G^{M,id}$, $\Delta \bar{G}_A^{M,id}$, $\Delta \bar{G}_B^{M,id}$, $\Delta S^{M,id}$, $\Delta \bar{S}_A^{M,id}$, and $\Delta \bar{S}_B^{M,id}$, where X_A is 0.4.

1.3 If A is 2 mole in Question 1.2, calculate $\Delta G'^{M,id}$ and $\Delta S'^{M,id}$.

1.1 By $\Delta G^{M,id} = x_A(RT\ln x_A) + x_B(RT\ln x_B)$ / $\Delta S^{M,id} = -x_A R\ln x_A - x_B R\ln x_B$





1.2

$\Delta G^{M,id} = 0.4\,(8.314 \times 900 \times \ln 0.4) + 0.6\,(8.314 \times 900 \times \ln 0.6) = -5035.88\ J/mol$ #

($8.314 \times 900 \times \ln 0.4 = \Delta \bar{G}_A^{M,id}$, $8.314 \times 900 \times \ln 0.6 = \Delta \bar{G}_B^{M,id}$)

$\Delta \bar{G}_A^{M,id} = -6856.24\ J/mol$, $\Delta \bar{G}_B^{M,id} = -3822.30\ J/mol$ #

$\Delta \bar{S}^{M,id} = 0.4 \cdot (-8.314 \cdot \ln 0.4) + 0.6\,(-8.314 \cdot \ln 0.6) = 5.60\ J/K \cdot mol$ #

($-8.314 \cdot \ln 0.4 = \Delta \bar{S}_A^{M,id}$, $-8.314 \cdot \ln 0.6 = \Delta \bar{S}_B^{M,id}$)

$\Delta \bar{S}_A^{M,id} = 7.62\ J/K \cdot mol$, $\Delta \bar{S}_B^{M,id} = 4.25\ J/K \cdot mol$ #

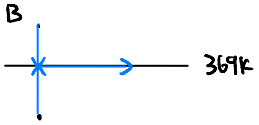
1.3 Mole of A is 2 mole

$X_A = 0.4$, total of mole is 5 mole

$\therefore\ \Delta G'^{M,id} = 5 \times (-5035.88) = -25179.4\ J$ #, $\Delta S'^{M,id} = 5 \cdot 5.60 = 28\ J/K$ #

2 A 2 mole of liquid A is at 300 K and a 3 mole of liquid B is at 400 K initially. Two liquid are mixed adiabatically, forming the ideal solution. The specific heat capacities of A and B are 100 and 150 J mol^{-1} K^{-1}, respectively. Calculate the change of entropy for whole process. Hint: Don't forget the effect from the temperature change.

By $\Delta H_A = \Delta H_B \Rightarrow 2 \cdot 100 \cdot (T-300) = 3 \cdot 150 \cdot (400-T) \Rightarrow T = 369.3\ K$



$dS = \frac{C_p}{T} dT$

$\Rightarrow \Delta S'_A = 2 \cdot \int_{300}^{369} \frac{100}{T} dT = 200 \ln\left(\frac{369}{300}\right) = 41.4\ J/K$

$\Delta S'_B = 3 \cdot \int_{400}^{369} \frac{150}{T} dT = 450 \ln\left(\frac{369}{400}\right) = -36.3\ J/K$

$\Delta S'^{M,id} = -R \cdot n \cdot (x_A \ln x_A + x_B \ln x_B) = -8.314 \cdot 5 \cdot [0.4 \ln 0.4 + 0.6 \ln 0.6] = 28.0\ J/K$

$\Delta S_{Total} = \Delta S'_A + \Delta S'_B + \Delta S'^{M,id} = 41.4 - 36.3 + 28.0 = \underline{33.1\ J/K}$ *

3 The activity coefficient of A in liquid A-B solution obeys the below relationship at 700 K.

$$\ln \gamma_A = X_B^2 - 0.2X_B^3 \rightarrow \ln a_A = x_B^2 - 0.2x_B^3 + \ln x_A$$

3.1 Is the solution positive deviation or negative deviation from Raoultian solution? Give the reason.

3.2 Derive the expression of $\ln \gamma_B$.

3.3 Draw the curves of a_A $vs.X_B$ and a_B $vs.X_B$.

3.1 Since $x_B \in [0,1]$, $x_B^2 - 0.2x_B^3 \in [0,1) \Rightarrow 0 \le \ln \gamma_A < 1 \Rightarrow 1 \le \gamma_A < e \approx 2.71828$

$\therefore$ Positive Raoultian Solution *

3.2 By G-D equation: $x_A d\ln\gamma_A + x_B d\ln\gamma_B = 0$, $\frac{d\ln\gamma_A}{dx_B} = 2x_B - 0.6x_B^2$

$\Rightarrow d\ln\gamma_B = -\frac{x_A}{x_B} d\ln\gamma_A = -x_A(2-0.6x_B)dx_B = x_A(2-0.6(1-x_A))dx_A$

$\Rightarrow \int_0^{\ln\gamma_B} d\ln\gamma_B = \int_0^{x_A} 1.4x_A + 0.6x_A^2 dx_A \Rightarrow \underline{\ln\gamma_B = 0.7x_A^2 + 0.2x_A^3}$ *

3.3