

# BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI

## Chemical Engineering Thermodynamics (CHE F213), Comprehensive Examination

Date – 21/12/2022

Part - A (Close Book)

Maximum Marks

60

1. Starting with the mathematical definition of partial molar property, derive the following: Summability equation relating mixture molar property and partial molar properties of its constituents

The Gibbs-Duhem equation

[5+3]

2. What is Gibb's theorem? Apply Gibb's theorem to derive expressions for entropy change and Gibbs energy change of mixing for ideal gas as a function of composition. [3+4+4]
3. 5 kg of oxygen and 2 kg of hydrogen are mixed at 1 atm and 25<sup>0</sup>C. Estimate the entropy change and Gibbs energy change of mixing (in SI units) assuming ideal behaviour. [4+4]
4. Vapor pressure expressions for three components in a ternary mixture are given as below:

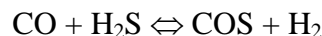
$$\ln P_1^{sat} = 14.3916 - \frac{2795.82}{T + 230}$$

$$\ln P_2^{sat} = 14.2724 - \frac{2945.27}{T + 224}$$

$$\ln P_3^{sat} = 14.2043 - \frac{2972.64}{T + 209}$$

In the above equations T is in <sup>0</sup>C and P<sup>sat</sup> is in kPa. Assuming that the system follows Rault's law, calculate total pressure (P), y<sub>1</sub>, y<sub>2</sub> and y<sub>3</sub> at T = 75<sup>0</sup>C and x<sub>1</sub> = 0.3 and x<sub>2</sub> = 0.4. x<sub>i</sub> and y<sub>i</sub> are mole fraction of component i in the liquid and vapor phase respectively. [5+3]

5. A pure gas obeys the two term virial equation of state  $\frac{PV}{RT} = 1 + \frac{BP}{RT}$ . The value of the second virial coefficient B = 1×10<sup>-4</sup> m<sup>3</sup>/mol. Determine the residual Gibbs energy and fugacity of this gas at 1000 kPa and 300 K. [4+3]
6. For a given binary system at constant temperature and pressure, the molar volume (in m<sup>3</sup>/mol) is given by  $V = 30x_A + 20x_B + x_Ax_B(15x_A - 7x_B)$  where x<sub>A</sub> and x<sub>B</sub> are the mole fractions of component A and B respectively. Compute the volume change of mixing at x<sub>A</sub> = 0.5. [6]
7. Carbon monoxide reacts with hydrogen sulphide at a constant temperature of 800 K and 2 bar as given below:



The standard Gibbs free energy of the reaction at 800 K is 22972.3 J/mol. All reactants and products can be assumed as ideal gases. If initially 1 mol of CO and 4 mol of H<sub>2</sub>S are present, determine the extent of reaction at equilibrium. [12]

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1. A binary mixture of acetone/1,3 Butadiene has acetone mole fraction of 0.28. compute volume and residual Gibbs energy of this mixture. **[30]**
2. The activity coefficients in a binary mixture of acetaldehyde(1)/methanol(2) are given by  $\ln\gamma_1 = 0.64x_2^2$  and  $\ln\gamma_2 = 0.64x_1^2$ . If this mixture forms an azeotrope at 320 K, compute the azeotropic composition. **[15]**
3. Consider the reaction  $\text{C}_2\text{H}_5\text{OH}(\text{g}) + (1/2)\text{O}_2(\text{g}) \rightarrow \text{CH}_3\text{CHO}(\text{g}) + \text{H}_2\text{O}(\text{g})$ .  
The reaction reaches equilibrium at 600<sup>0</sup>C and 1 bar. Assuming that the standard heat of this reaction is independent of temperature, Compute the value of equilibrium constant at 600<sup>0</sup>C and 1 bar. **[15]**