INSA | INSTITUT NATIONAL
DES SCIENCES
APPLIQUÉES
LYON

FC – AMERINSA – ASINSA - EURINSA – SCAN –SHN

Monday, the 2nd of December 2024

WRITTEN TEST OF CHEMISTRY 2 (2 h)

- *No document allowed. Any type of calculator allowed.*
- *Gases are assumed to behave as ideal gases.*
- *For the calculations, use:*

$$R = 8.314 \, J \cdot mol^{-1} \cdot K^{-1} \, ; 0 \, °C = 273 \, K$$

$$1 \, atm = 760 \, mm \, Hg = 760 \, Torr = 101 \, 325 \, Pa = 1.01325 \, bar,$$

- *The influence of temperature on enthalpy and entropy changes is neglected.*
- *Your answers and your approach must be concisely justified. Literal formulas must clearly appear, then put into numerical form before giving the result of your calculations.*

Exercise I: Isobaric diagram for water/benzene (with P= 1.00 bar) (13 points)

Benzene is an organic solvent whose use is currently highly regulated.
We propose to establish the isobaric (at P = 1.00 bar) liquid-vapor (L-V) phase diagram of a binary mixture of water (compound 1) and benzene (compound 2), water and benzene being considered totally immiscible.

I.1 Justify that water-benzene mixtures can be considered completely immiscible, based on the structure and respective properties of the two molecules. Does this mixture obey the ideal solution model?

I.2 Using the data provided, calculate, under total pressure P = 1.00 bar, the coordinates of the heteroazeotrope (H) of the water-benzene mixture. T_H will be calculated to within +/- 1 K, and x_H (expressed as the mole fraction of benzene) to within +/-0.01.

I.3 Note x_2 the mole fraction of benzene in the liquid phase and y_2 the mole fraction of benzene in the vapor phase, respectively. Using the data calculated in I.2 and those in Table 1, plot the isobaric Liquid-Vapor (L-V) phase diagram of the binary mixture of water-benzene at P = 1.00 bar on the graph paper supplied with the text.

I.4. List the phases available at the boiling temperature of the heteroazeotrope. What are the special features of mixtures with zero miscibility?

I.5 At P = 1.00 bar, a gaseous mixture with a mole fraction of benzene y_2 = 0.90 is cooled. Indicate the temperature at which the liquid appears, and the temperature at which the vapor disappears.

I.6 An equimolar liquid mixture of water and benzene is heated at P = 1.00 bar.

I.6.1 At what temperature does boiling begin? What is the composition of the vapor phase?

I.6.2 The obtained vapor is eliminated as it is formed, using the method seen during the labwork. Indicate which liquid phase disappears first. What is the temperature when this liquid disappears? What is then the composition of the vapor phase?

I.6.3 Schematize the experimental set-up used to perform this operation.

I.6.4 Indicate a practical advantage of distilling an immiscible mixture of water and another pure substance with the same type of liquid-vapor diagram as the water-benzene mixture.

I.7 A mixture of water and benzene consisting of 25.2 g water and 46.8 g benzene is introduced into a closed vessel at 25°C, under total pressure P = 1.00 bar.

Indicate the exact composition of the system at equilibrium (nature of the phases, number of moles (to within +/-0.1 mole) and weight (to within +/-0.1g) of each component in each phase for the following temperatures:

a) T = 330 K
b) T = 357 K
c) T = 370 K
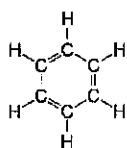
Present your results in a table.

Data:

Water: Clapeyron's equation : $\ln P^*_{water(bar)} = \dfrac{-5292.3}{T} + 14.169$

Molar mass: 18 g. mol^{-1}

Benzene :

Boiling temperature at P = 1.00 bar: 353 K.

Enthalpy of vaporization $\overline{\Delta_{vap}H^0}$ = 32.426 kJ $\cdot$ mol^{-1}

Molar mass: 78 g. mol^{-1}

Table 1: *temperature T at which a liquid phase appears during cooling as a function of the initial composition $y_{2(init)}$ of a vapor phase (mole fraction of benzene) for P* = 1.00 bar.

$y_{2(init)}$	0.10	0.30	0.50	0.70	0.80	0.90
T (K)	370	364	357	345	348	352

Exercise II: Synthesis of dihydrogen through dissociation of water (7 points)

We would like to investigate the possibility of producing dihydrogen from gaseous water. Indeed, water can dissociate into dioxygen and dihydrogen according to the following equilibrium:

$$2\,H_2O_{(g)} \rightleftarrows 2\,H_2\,_{(g)} + O_{2(g)}$$
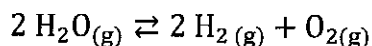
II.1 Will a rise in temperature favor the production of H_2?
Same question with a rise in pressure.

II.2 Define the notions of dissociation coefficient of a reactant on a one hand, and the yield of a product on the other hand, at equilibrium.

II.3 The initial system consists of 2 mol of water. With the use of a detailed table of advancement, express the equilibrium constant $K°_T$ as a function of the yield in H_2, noted r, and the total pressure P.

II.4 Calculate the equilibrium constant $K°_T$ at $T = 1000$ K.

II 5 Calculate the yield r under $P = 1$ bar and at $T = 1000$ K. The algebraic calculation of r requires to set a simplifying assumption, that requires to be then verified.

II. 6 Calculate the temperature at which, at equilibrium, 30 % of the molar quantity of gaseous water initially introduced would theoretically be consumed, assuming a constant pressure $P = 1$ bar. What would then be the molar composition of the gaseous mixture at equilibrium?

II. 7 Calculate the total pressure P' under which, at equilibrium at $T = 1000$ K, 30 % of the molar quantity of gaseous water initially introduced would theoretically be consumed.

II.8 Would the addition of an inert gas with respect to the reaction, increase the yield in H_2, assuming that the total pressure P remains constant?
Same question if we work at constant volume. Qualitatively justify your answers

II.9 Given the results obtained in the previous questions, is it technically and economically feasible to produce dihydrogen H_2 according to the given reaction?

Name another way of obtaining dihydrogen.

Data :

Compound	$\Delta_f H_{298}^0$ (kJ $\cdot$ mol^{-1})	S_{298}^0 (J $\cdot$ K^{-1} $\cdot$ mol^{-1})
$H_2O_{(g)}$	-250.9	198.3
$H_2\,_{(g)}$	0	130.6
$O_2\,_{(g)}$	0	204.8