Answer Sheet for CHE654 Homework Set #3
(100 points)

19. (20 points) ***Using ASPEN Plus to Perform Basic Calculations***

(a) Calculate the bubble-point temperature in °C of a mixture containing 30 mol% benzene, 30 mol% cyclohexane, 20 mol% toluene, and 20 mol% *n*-octane at 1.01325 bar. Use PENG-ROB as the property method.

Answer: T_{BUBBLE} = _____ °C

(b) Calculate the solubility of 1-pentanol in water in terms of mole% when we mix 1.0 lbmol of 1-pentanol with 1.0 lbmol of water at 14.7 psia and 100 °F. Use UNIQUAC as the property method.

Answer: Solubility (mol%) of 1-pentanol in water = _____ mol%

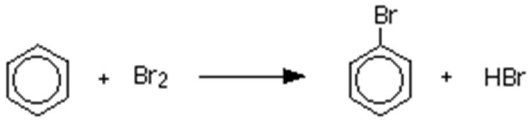
(c) Determine the solubility in ppm-mole of argon gas in water when we mix 1.0 lbmol of argon with 10.0 lbmol of water at 50 °F and 14.7 psia. Use IDEAL with Henry's Law as the property method.

Answer: Solubility of argon in water = _____ ppm (mole)

(d) Determine the temperature in °C at which a mixture of 20 mol% acetone, 30 mol% ethanol, and 50 mol% water at 1.01325 bar gives rise to a vapor stream with 50 mol% of acetone. Use NRTL-RK as the property method.

Answer: T = _____ °C

(e) The reaction between benzene and bromine in the presence of either aluminium bromide or iron gives bromobenzene as follows.



Calculate the heat of reaction ΔH_{rxn} of this gas-phase reaction at 200°C and 1 bar, based on one gmole of each reactant and assuming 100% conversion. Determine if the reaction is endothermic or exothermic. Use PENG-ROB as the property method.

Answer: ΔH_{rxn} = _____ cal/gmol (Circle one: endothermic or exothermic)

20. (20 points) ***Simulation of a Cyclohexane Production Process***

Answer the following questions:

1. Pressure of the column condenser = _____ psia
2. Purge fraction = _____
3. Temperature of the flash vessel = _____ °F
4. Purity of cyclohexane (mole%) in the product stream = _____ %

22. (30 points) ***Solving a Highly Constrained Cumene Production Problem***

Answer the following questions:

1. Temperature of the condenser in BZ-COL = _____ °F
2. Molar ratio of propylene to benzene in the reactor inlet (REAC-IN) = _____
3. Reactor length = _____ feet

23. (30 points) ***Solving a Highly Constrained Bromobenzene/1-Bromocyclohexane Production Problem***

Answer the following questions:

Distillate % mole recovery of Light Key in Column 2 = _____ mol%

Purity of bromobenzene in the distillate overhead of Column 3 = _____ mol%

Purity of cyclohexyl-bromide in the bottom stream of Column 3 = _____ mol%

Distillate vapor fraction in Column 2 = _____

Split fraction going to PURGE = _____