Solution

ChE 3063 **Project 3** Due: December 6, 2013

Benzene can be produced from n-hexane by the following gas phase reactions:

C_6H_{14}	⇆	C_6H_{12} +	H_2	rxn 1)
n-hexane		1-hexene		
C_6H_{12}	⇆	C_6H_6 +	$3H_2$	rxn 2)
1-hexene		benzene		

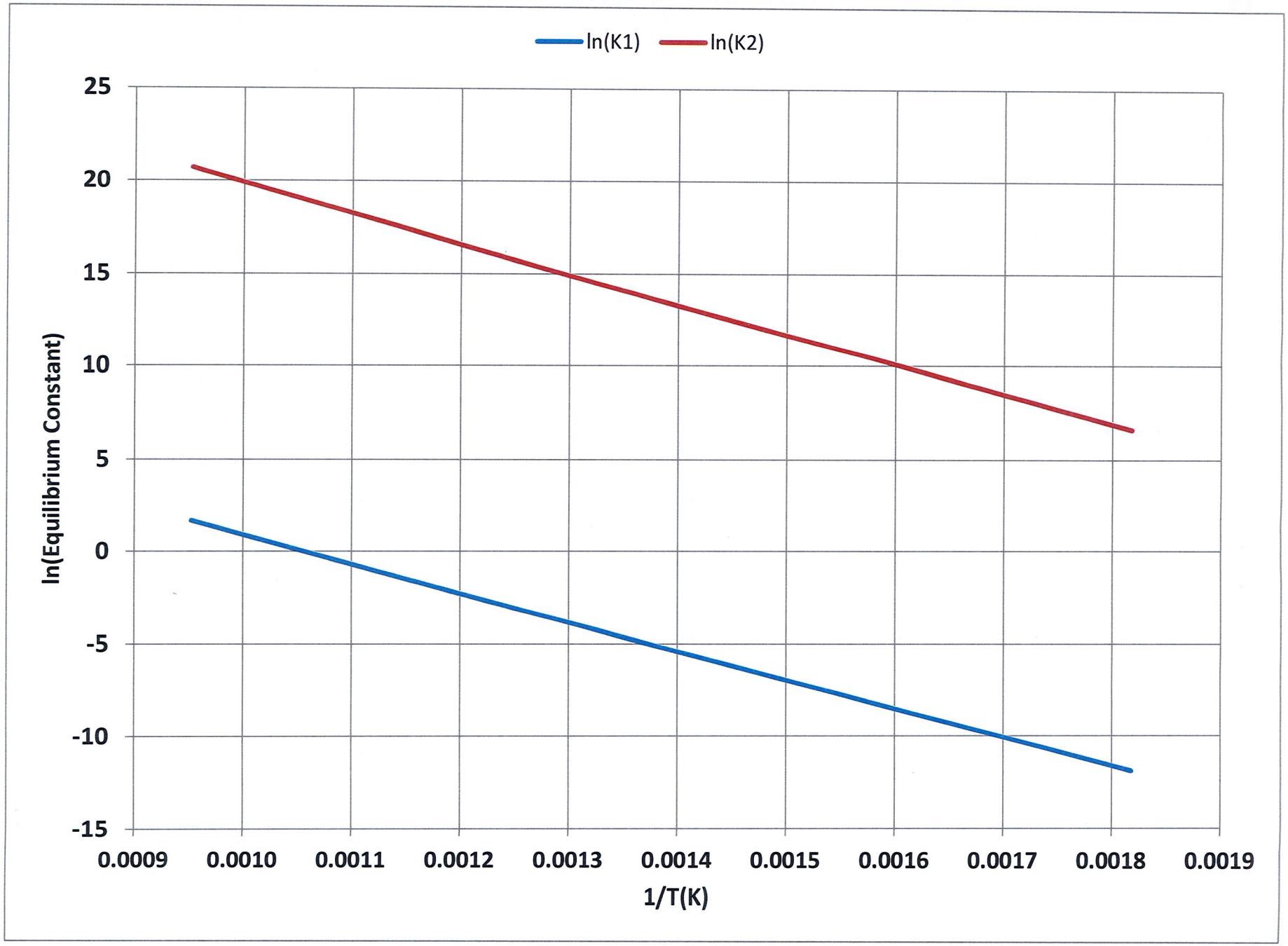
These reactions represent a very small fraction of the important refinery process called reforming where naptha, which are C_5 - C_8 or so paraffins, are converted to aromatics on a platinum catalyst. The thermodynamic features of the process are largely represented by the reactions given above. High temperatures are necessary to make the reactions thermodynamically favorable. In order to properly operate the catalyst, we need high hydrogen partial pressures to stop coke formation even though the forward reaction is favored by low hydrogen partial pressures. Therefore, we usually co-feed hydrogen with the hexane reactant. We need equilibrium data in the range 550-1050K at 10 bar and 25 bar total pressure.

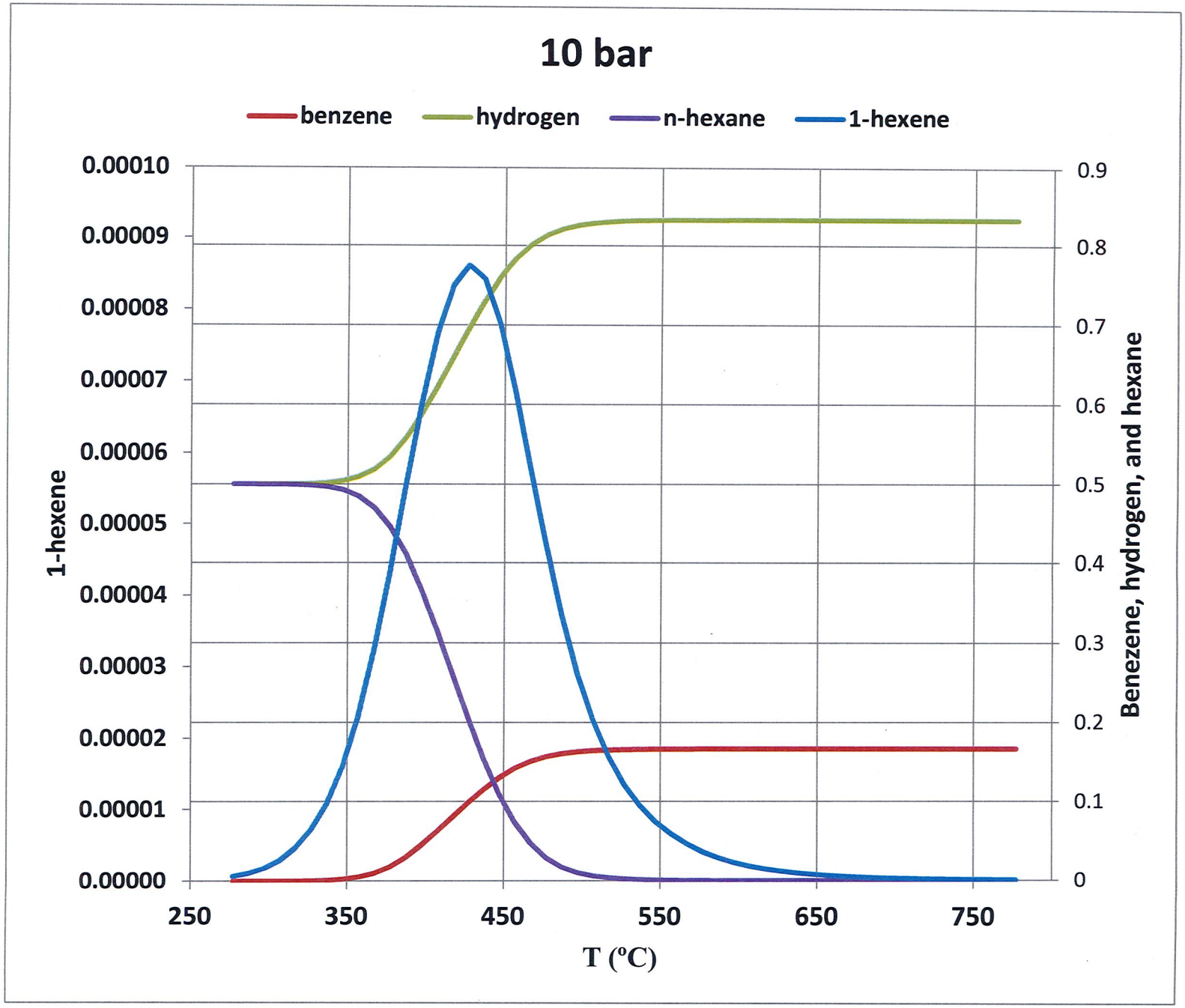
A. Calculate and plot $\ln(K_a)$ vs 1/T (°K) for each pressure, for each reaction.

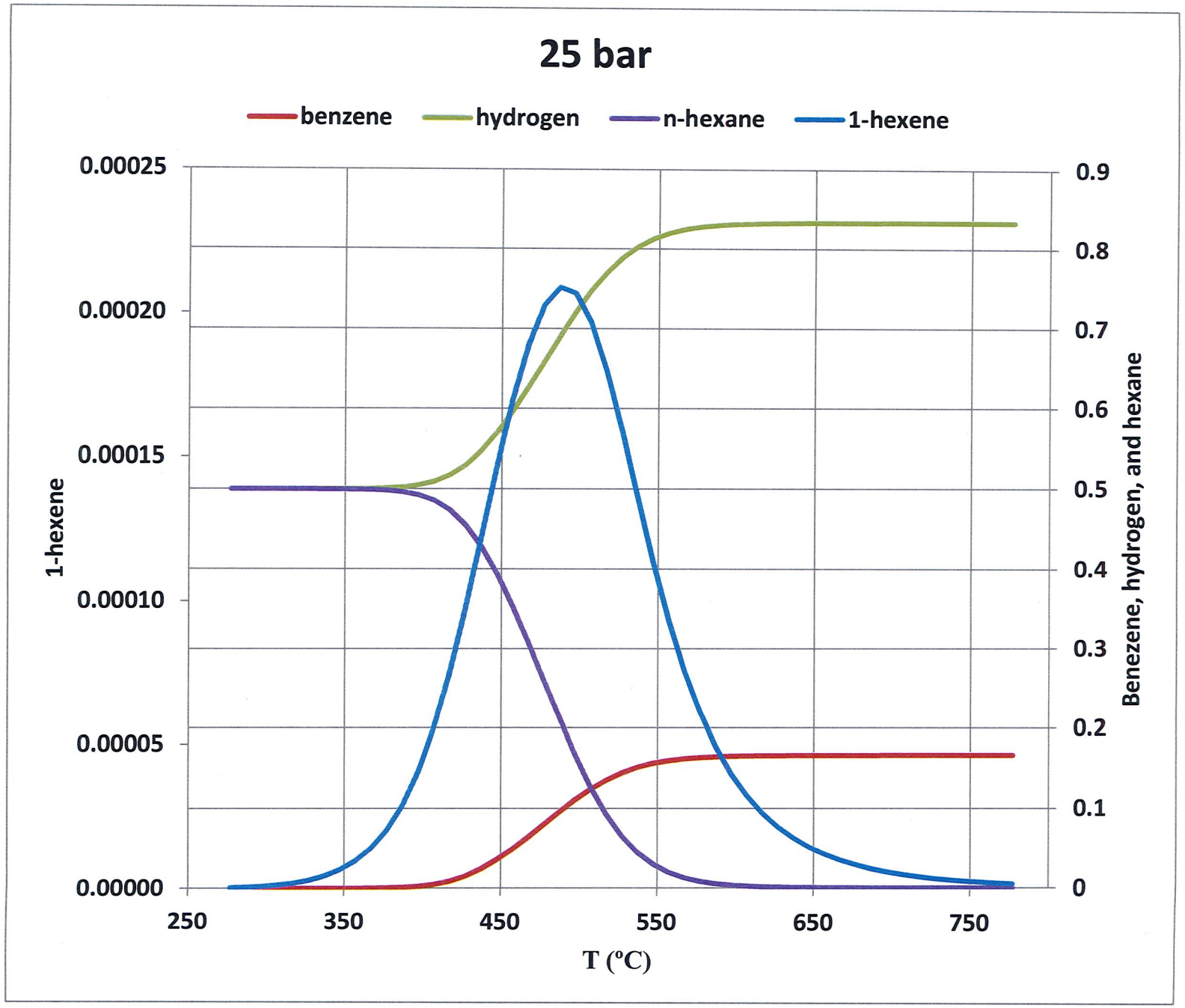
B. Calculate and plot the mole fraction of each species (n-hexane, 1-hexene, benzene, and hydrogen) at equilibrium for each pressure as a function of temperature for an initial mixture which contains 1 mole n-hexane and 1 mole H_2 with no other products.

Notes:

When preparing your plots, especially the plot from part B), note that several orders of magnitude may separate some of the curves of interest. In that case, set up a second axis with a different scale to better show the components that are in low concentrations.


ln(K1)
ln(K2)
25
20
15
10
5
0
-5
-10
-15
ln(Equilibrium Constant)
0.0009
0.0010
0.0011
0.0012
0.0013
0.0014
0.0015
0.0016
0.0017
0.0018
0.0019
1/T(K)


10 bar
benzene
hydrogen
n-hexane
1-hexene
0.00010
0.00009
0.00008
0.00007
0.00006
0.00005
0.00004
0.00003
0.00002
0.00001
0.00000
1-hexene
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Benezene, hydrogen, and hexane
250
350
450
550
650
750
T (°C)


25 bar
benzene
hydrogen
n-hexane
1-hexene
0.00025
0.00020
0.00015
0.00010
0.00005
0.00000
1-hexene
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Benezene, hydrogen, and hexane
250
350
450
550
650
750
T (°C)