SOLUTION

ChE 3063 **EXAM III** **November 14, 2014**

Open Books and Notes

The Diels-Alder addition of 1,3 butadiene to propylene yields methylcyclohexene:

or B + P $\rightarrow$ MCH

Note that there is no heat capacity, enthalpy of formation, or free energy of formation data for MCH in your text book, though data for 1,3 butadiene and propylene do appear in your book.

To simplify your calculations, you may treat C_p's as constant with temperature. Values to be used are:

$C_{p,B} = 89.13$ J/mole-K $\quad$ $C_{p,P} = 64.78$ J/mole-K $\quad$ $C_{p,MCH} = 116.40$ J/mole-K

For all calculations you may assume ideal gases.

A) 15 points

At 298 K and P = 10 bar, an equilibrium mixture of B, P, and MCH was $y_B^E = 0.110$, $y_P^E = 0.110$, $y_{MCH}^E = 0.780$. Find K_a and ΔG°_R at 298K.

B) 15 points

Find $\Delta G^\circ_{f,298,MCH}$ (the free energy of formation for MCH at 298K)

C) 10 points

How is the equilibrium constant for the reverse reaction (call it K_{ar}): MCH $\rightarrow$ B + P related to the equilibrium constant for the forward reaction (call it K_{af}) at the same temperature?

D) 20 points

Given that at 308K and P = 10 bar, an equilibrium mixture of B, P, and MCH was $y_B^E = 0.180$, $y_P^E = 0.180$, $y_{MCH}^E = 0.640$, estimate ΔH°_R for the temperature range 298 - 308 K assuming ΔH°_R is approximately constant for this small T range.

E) 40 points

Estimate ΔH°_R, ΔS°_R, and ΔG°_R at 200°C for this reaction.