ChE 3063 Exam III Nov. 12, 2018

Solution

I. $C_8H_{10} \rightarrow C_8H_8 + H_2$

		C_8H_{10}	C_8H_8	H_2
J/m	$\Delta H^\circ_{f,298}$	29,420	147,360	0
J/m	$\Delta G^\circ_{f,298}$	130,890	213,900	0
J/mK	$\Delta S^\circ_{f,298}$	-338.7	-223.2	0
	a	1.124	2.050	3.249
	$bx10^3$	55.380	50.192	0.422
	$cx10^6$	-18.476	-16.662	0
	$dx10^{-5}$	0	0	0.083
	ΔA	4.175		
	ΔB	-0.00466		
	ΔC	$1.814x10^{-6}$		
	ΔD	8300		

at 298, $\Delta H^\circ_{R,298} = 117440.0$ J/m

$\Delta S^\circ_{R,298} = 115.48$ J/m·K

$\Delta G^\circ_{R,298} = 83010.0$

at 700°C = 973.15 K

$$\Delta H^\circ_{R,973} = \Delta H^\circ_{R,298} + \int_{298}^{973} C_p^{IG}\, dT$$

$$\Delta S^\circ_{R,973} = \Delta S^\circ_{R,298} + \int_{298}^{973} C_p^{IG} \frac{dT}{T}$$

$\Delta H^\circ_{R,973} = 117440.0 + 11088.6 = 128528.6$ J/m

$\Delta S^\circ_{R,973} = 115.48 + 21.1 = 136.6$ J/m·K

$\Delta G^\circ_{R,973} = \Delta H^\circ_{R,973} + 973\Delta S^\circ_{R,973} = -4419.81$ J/m

a) $K_{eq} = \exp\left(\frac{4419.81}{8.314 \cdot 973.15K}\right) = 1.72681$

b)

	Start	Finish
C_8H_{10}	1	$1-\xi$
C_8H_8	0	ξ
H_2	1	$1+\xi$
	2	$2+\xi$

$$y_{C_8H_{10}} = \frac{1-\xi}{2+\xi}$$

$$y_{C_8H_8} = \xi/(2+\xi)$$

$$y_{H_2} = 1+\xi/(2+\xi)$$

c) $K_a = K_y P^{\Sigma\nu_i} = \dfrac{\left(\frac{\xi}{2+\xi}\right)\left(\frac{1+\xi}{2+\xi}\right)}{\left(\frac{1-\xi}{2+\xi}\right)} 5\ bar$

$$K_a = \frac{(\xi)(1+\xi)}{(1-\xi)(2+\xi)} 5 = 1.72681$$

$$\xi = 0.374$$

$$y_{C_8H_{10}} = 0.26383$$
$$y_{C_8H_8} = 0.1574$$
$$y_{H_2} = 0.5787$$