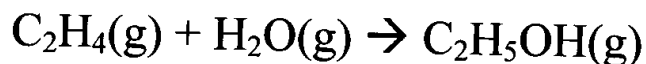


CH302H – Principles of Chemistry II: Honors
Fall 2014, Unique 51880

Quiz 3, 27 February 2014

One way to produce ethanol (if you don't have any corn and a still handy) is from the reaction of ethene gas and water vapor:



Describe, both qualitatively and quantitatively, the optimum conditions of pressure and temperature necessary to make as much ethanol in this process as possible.

The following information may be useful:

	ΔH_f° (kJ mol ⁻¹)	S_m° (J K ⁻¹ mol ⁻¹)	ΔG_f° (kJ mol ⁻¹)
C ₂ H ₄ (g)	52.3	219.5	68.1
H ₂ O(g)	-241.8	188.7	-228.6
C ₂ H ₅ OH(g)	-235.1	282.6	-168.6

$$\Delta G_{\text{rxn}}^\circ = \sum_{\text{prod}} \nu \Delta G_f^\circ - \sum_{\text{react}} \nu \Delta G_f^\circ = \Delta G_f^\circ(\text{EtOH}) - \Delta G_f^\circ(\text{C}_2\text{H}_4) - \Delta G_f^\circ(\text{H}_2\text{O})$$

$$\Delta G_{\text{rxn}}^\circ = -168.6 \text{ kJ/mol} - 68.1 \text{ kJ/mol} - (-228.6 \text{ kJ/mol}) = -8.1 \text{ kJ/mol}$$

$$\Delta H_{\text{rxn}}^\circ = \Delta H_f^\circ(\text{EtOH}) - \Delta H_f^\circ(\text{C}_2\text{H}_4) - \Delta H_f^\circ(\text{H}_2\text{O}) = -235.1 \text{ kJ/mol} - 52.3 \text{ kJ/mol} - (-241.8 \text{ kJ/mol}) = -45.6 \text{ kJ/mol}$$

$$\Rightarrow k_p = \exp\left[-\frac{\Delta G_{\text{rxn}}^\circ}{RT}\right] = \exp\left[-\frac{-8.1 \times 10^3 \text{ J/mol}}{(8.314 \text{ J/mol}\cdot\text{K})(298 \text{ K})}\right] = 26.3$$

Pressure: Qualitatively, Le Chatelier tells us that if we increase pressure we will drive the rxn to the side w/ the fewest moles of gas, which in this case is the products. So we should increase P.

Quantitatively: $k_p = k_x P_{\text{TOT}}^{\sum \nu_i} = k_x P_{\text{TOT}}^{-1-1} = \frac{k_x}{P_{\text{TOT}}}$



Quiz 3, cont.

Let's say we want to increase the amount of products so they outnumber reactants by 100x (instead of 26.3x w/ this k_p)

$$k_x = 100 \Rightarrow P_{TOT} = \frac{k_x}{k_p} = \frac{100}{26.3} = \underline{3.8}$$

So I should increase P_{TOT} by a factor of 3.8 by reducing volume of the rxn vessel containing this rxn.

Temperature: Qualitative: Le Chatelier says that since $\Delta H_{rxn} < 0$, that if I decrease temperature, I will drive the rxn to the desired product side.

Quantitative: Again, let's say I want to make product outnumber reactants by 100x, i.e. $k_p(T_2) = 100$

$$\ln\left(\frac{k_p(T_2)}{k_p(T_1)}\right) = \frac{-\Delta H_{rxn}^\circ}{R} \left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$\text{Solve for } T_2: \frac{1}{T_2} = \frac{-R}{\Delta H_{rxn}^\circ} \ln\left(\frac{k_p(T_2)}{k_p(T_1)}\right) + \frac{1}{T_1} = \frac{-(8.314 \text{ J/kmol})}{(-45.6 \times 10^3 \text{ J/mol})} \ln\left(\frac{100}{26.3}\right) + \frac{1}{298 \text{ K}}$$

$$\frac{1}{T_2} = 0.0036 \text{ 1/K}$$

$$\boxed{T_2 = 278 \text{ K}} \quad \text{cool to } 278 \text{ K}$$

*Note - these exact answers depended on our use of $k_x = k_p(T_2) = 100$. We