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:

$$C_2H_4(g) + H_2O(g) \rightarrow C_2H_5OH(g)$$

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^0_f (kJ mol^{-1})	S^0_m (J K^{-1} mol^{-1})	ΔG^0_f (kJ mol^{-1})
$C_2H_4(g)$	52.3	219.5	68.1
$H_2O(g)$	-241.8	188.7	-228.6
$C_2H_5OH(g)$	-235.1	282.6	-168.6

$$\Delta G^\circ_{rxn} = \sum_{prod} \nu \Delta G^\circ_f - \sum_{react} \nu \Delta G^\circ_f = \Delta G^\circ_f(EtOH) - \Delta G^\circ_f(C_2H_4) - \Delta G^\circ_f(H_2O)$$

$$= -168.6 \text{ kJ/mol} - 68.1 \text{ kJ/mol} - {}^{-}228.6 \text{ kJ/mol}$$

$$\underline{\Delta G^\circ_{rxn} = -8.1 \text{ kJ/mol}} \Rightarrow K_p = \exp\left[-\frac{\Delta G^\circ_{rxn}}{RT}\right] = \exp\left[\frac{-{}^{-}8.1\times10^3 \text{ J/mol}}{(8.314 \text{ J/K mol})(298 \text{ K})}\right] = \underline{26.3}$$

$$\Delta H^\circ_{rxn} = \Delta H^\circ_f(EtOH) - \Delta H^\circ_f(C_2H_4) - \Delta H^\circ_f(H_2O) = -235.1 \text{ kJ/mol} - 52.3 \text{ kJ/mol} - {}^{-}241.8 \text{ kJ/mol}$$

$$\underline{\Delta H^\circ_{rxn} = -45.6 \text{ kJ/mol}}$$

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: $K_p = K_x P_{TOT}^{\sum \nu_i} = K_x P_{TOT}^{1-1-1} = \frac{K_x}{P_{TOT}}$

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Quiz 3, cont.

Let's say we want to increase the amount of products so they outnumber reactants by 100 x (instead of 26 x w/ this K_p)

$K_x = 100 \Rightarrow \qquad P_{TOT} = \frac{K_x}{K_p} = \frac{100}{26.3} = \underline{3.8}$

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 $\Delta H^\circ_{rxn} < 0$, 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. $K_p(T_2) = 100$

$$\ln\left(\frac{K_p(T_2)}{K_p(T_1)}\right) = \frac{-\Delta H^\circ_{rxn}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

Solve for T_2: $\frac{1}{T_2} = \frac{-R}{\Delta H^\circ_{rxn}} \ln\left(\frac{K_p(T_2)}{K_p(T_1)}\right) + \frac{1}{T_1} = \frac{-(8.314\,\text{J/K mol})}{(-45.6\times10^3\,\text{J/mol})} \ln\left(\frac{100}{26.3}\right) + \frac{1}{298\,\text{K}}$

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

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

*note - these exact answers depended on our use of $K_x = K_p(T_2) = 100$. We