Solution to Exam 4 CM205, 5/11/2000

1. **Heat of formation for nitrogen dioxide:** $\Delta H_f := 33.8$ **kJ/mol**

Heat capacities:

$$C_{pNO2}(T) := 0.03607 + 3.97\cdot 10^{-5}\cdot T - 2.88\cdot 10^{-8}\cdot T^2 + 7.87\cdot 10^{-12}\cdot T^3$$

$$C_{pN2}(T) := 0.029 + 0.2199\cdot 10^{-5}\cdot T + 0.5723\cdot 10^{-8}\cdot T^2 - 2.871\cdot 10^{-12}\cdot T^3$$

$$C_{pO2}(T) := 0.0291 + 1.158\cdot 10^{-5}\cdot T - 0.6076\cdot 10^{-8}\cdot T^2 + 1.311\cdot 10^{-12}\cdot T^3$$

Reaction: $\left(\frac{1}{2}\cdot N_2 + O_2\right) = \left(NO_2\right)$

$$\Delta H := \int_{100}^{25}\left(C_{pO2}(T) + \frac{1}{2}\cdot C_{pN2}(T)\right)dT + \Delta H_f + \int_{25}^{100} C_{pNO2}(T)\,dT$$

$\Delta H = 33.354$ **kJ/mol**

2 $\Delta H_r = \Delta H_{f,AB2,aq} - 2\cdot\left(\Delta H_{f,B,aq}\right) - \Delta H_{f,A,aq} = 110\cdot\frac{kJ}{mol}$

$$\Delta H_{f,AB2,aq} = -120 + \Delta H_{m,AB2,\infty}$$

$$\Delta H_{f,B,aq} = -50 - 35 = -85$$

$$\Delta H_{f,A,aq} = -100 - 20 = -120$$

$$\Delta H_{m,AB2,\infty} = 110 - 2\cdot 85 - 120 + 120 = -60\cdot\frac{kJ}{mol\cdot AB_2}$$

3. $Mg + O_2 + H_2 \rightarrow Mg(OH)_2$

4. $C_7H_8O(l) + (17/2)\ O_2(g) \rightarrow 7CO_2(g) + 4H_2O(l)$

5. **Basis: 100 mols of ethylene oxide**

$n_{C2H4Oout} := 100$ $\quad n_{CO2out} := \frac{9.2}{6.9}\cdot 100$ $\quad n_{H2Oout} := \frac{9.2}{6.9}\cdot 100$

$n_{rxn1} := 100$ $\quad n_{rxn2} := \frac{n_{H2Oout}}{2}$ $\quad n_{rxn2} = 66.667$

$n_{C2H4in} := n_{rxn1} + n_{rxn2}$

$$n_{O2out} + n_{N2out} = \frac{100 - (6.9 + 9.2 + 9.2)}{6.9}\cdot 100$$

$$n_{N2in} = n_{N2out}$$

$$n_{O2in} = \frac{21}{79} \cdot n_{N2in} = \frac{21}{79} \cdot n_{N2out} = \frac{1}{2} \cdot n_{rxn1} + 3 \cdot n_{rxn2} + n_{O2out}$$

or $$\frac{21}{79} \cdot n_{N2out} - n_{O2out} = \frac{1}{2} \cdot n_{rxn1} + 3 \cdot n_{rxn2} = 250$$

Solving the following simultaneously,

$$n_{O2out} + n_{N2out} = \frac{100 - (6.9 + 9.2 + 9.2)}{6.9} \cdot 100$$

$$\frac{21}{79} \cdot n_{N2out} - n_{O2out} = \frac{1}{2} \cdot n_{rxn1} + 3 \cdot n_{rxn2} = 250$$

$$n_{N2out} := \frac{\left[\frac{100 - (6.9 + 9.2 + 9.2)}{6.9} \cdot 100\right] + 250}{1 + \frac{21}{79}}$$

$$n_{N2in} := n_{N2out}$$

$$n_{O2in} := \frac{21}{79} \cdot n_{N2in}$$

$$n_{O2out} := n_{O2in} - 250$$

In summary,

$n_{C2H4Oout} := 100$ $\quad$ $n_{C2H4in} = 166.667$

$n_{CO2out} = 133.333$ $\quad$ $n_{N2in} = 1.053 \cdot 10^{3}$

$n_{H2Oout} = 133.333$ $\quad$ $n_{O2in} = 279.848$

$n_{N2out} = 1.053 \cdot 10^{3}$

$n_{O2out} = 29.848$

b) Heats of reaction:

$$\Delta H_{rxn1} := (-51) - (52.28)$$

$$\Delta H_{rxn2} := (2 \cdot (-393.5) + 2 \cdot (-241.83)) - (52.28)$$

Heat capacities:

$$C_{pCO2}(T) := 0.03611 + 4.233 \cdot 10^{-5} \cdot T - 2.887 \cdot 10^{-8} \cdot T^2 + 7.464 \cdot 10^{-12} \cdot T^3$$

$$C_{pN2}(T) := 0.029 + 0.2199 \cdot 10^{-5} \cdot T + 0.5723 \cdot 10^{-8} \cdot T^2 - 2.871 \cdot 10^{-12} \cdot T^3$$

$$C_{pH2O}(T) := 0.03346 + 0.688 \cdot 10^{-5} \cdot T + 0.7604 \cdot 10^{-8} \cdot T^2 - 3.593 \cdot 10^{-12} \cdot T^3$$

$$C_{pC2H4}(T) := 0.04075 + 11.47 \cdot 10^{-5} \cdot T - 6.891 \cdot 10^{-8} \cdot T^2 + 17.66 \cdot 10^{-12} \cdot T^3$$

$$C_{pO2}(T) := 0.0291 + 1.158\cdot 10^{-5}\cdot T - 0.6076\cdot 10^{-8}\cdot T^2 + 1.311\cdot 10^{-12}\cdot T^3$$

$$C_{pC2H4O}(T) := 0.441\cdot 10^{-3} + 0.151\cdot 10^{-5}\cdot T - 9.995\cdot 10^{-8}\cdot T^2$$

Cool feed down from 200 to 25:

$$dh_1 := \int_{200}^{25} n_{O2in}\cdot C_{pO2}(T)\, dT \qquad dh_1 = -1.485\cdot 10^3$$

$$dh_2 := \int_{200}^{25} n_{N2in}\cdot C_{pN2}(T)\, dT \qquad dh_2 = -5.403\cdot 10^3$$

$$dh_3 := \int_{200}^{25} n_{C2H4in}\cdot C_{pC2H4}(T)\, dT \qquad dh_3 = -1.536\cdot 10^3$$

React:

$$dh_4 := n_{rxn1}\cdot \Delta H_{rxn1} \qquad dh_4 = -1.033\cdot 10^4$$

$$dh_5 := n_{rxn2}\cdot \Delta H_{rxn2} \qquad dh_5 = -8.82\cdot 10^4$$

Heat products to 600:

$$dh_6 := \int_{25}^{600} n_{CO2out}\cdot C_{pCO2}(T)\, dT \qquad dh_6 = 3.538\cdot 10^3$$

$$dh_7 := \int_{25}^{600} n_{O2out}\cdot C_{pO2}(T)\, dT \qquad dh_7 = 549.747$$

$$dh_8 := \int_{25}^{600} n_{N2out}\cdot C_{pN2}(T)\, dT \qquad dh_8 = 1.831\cdot 10^4$$

$$dh_9 := \int_{25}^{600} n_{H2Oout}\cdot C_{pH2O}(T)\, dT \qquad dh_9 = 2.788\cdot 10^3$$

$$dh_{10} := \int_{25}^{600} n_{C2H4Oout}\cdot C_{pC2H4O}(T)\, dT \qquad dh_{10} = -667.098$$

$$Q := dh_1 + dh_2 + dh_3 + dh_4 + dh_5 + dh_6 + dh_7 + dh_8 + dh_9 + dh_{10}$$

$Q = -8.243\cdot 10^4$ **kJ/hr**

6. $C_7H_{16} + 15/2\ O_2 \rightarrow 7CO(g) + 8H_2O(g)$

$$\Delta H_r := (7\cdot(-110.52) + 8\cdot(-241.83)) - (-224.4)$$

$$\Delta H_r = -2.484\cdot 10^3$$ kJ/mol

Alternatively, using combustion reaction of heptane and CO and water evaporation,

$$\Delta H_r := (-4816.9) - 7\cdot(-282.99) + 8\cdot(-241.83 + 285.84)$$

$$\Delta H_r = -2.484\cdot 10^3$$ kJ/mol