

Solution to Exam 4 CM205, 5/11/2000

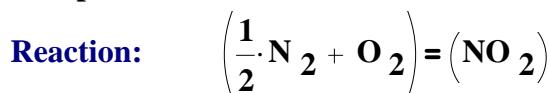
1. Heat of formation for nitrogen dioxide: $\Delta H_f = 33.8 \text{ kJ/mol}$

Heat capacities:

$$C_{pNO_2}(T) := 0.03607 + 3.97 \cdot 10^{-5} \cdot T - 2.88 \cdot 10^{-8} \cdot T^2 + 7.87 \cdot 10^{-12} \cdot T^3$$

$$C_{pN_2}(T) := 0.029 + 0.2199 \cdot 10^{-5} \cdot T + 0.5723 \cdot 10^{-8} \cdot T^2 - 2.871 \cdot 10^{-12} \cdot T^3$$

$$C_{pO_2}(T) := 0.0291 + 1.158 \cdot 10^{-5} \cdot T - 0.6076 \cdot 10^{-8} \cdot T^2 + 1.311 \cdot 10^{-12} \cdot T^3$$



$$\Delta H := \int_{100}^{25} \left(C_{pO_2}(T) + \frac{1}{2} \cdot C_{pN_2}(T) \right) dT + \Delta H_f + \int_{25}^{100} C_{pNO_2}(T) dT$$

$$\Delta H = 33.354 \text{ kJ/mol}$$

$$2 \quad \Delta H_r = \Delta H_{f, AB_2, aq} - 2 \cdot (\Delta H_{f, B, aq}) - \Delta H_{f, A, aq} = 110 \cdot \frac{\text{kJ}}{\text{mol}}$$

$$\Delta H_{f, AB_2, aq} = -120 + \Delta H_{m, AB_2, \infty}$$

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

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

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



5. Basis: 100 mols of ethylene oxide

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

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

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

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

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

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

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

Solving the following simultaneously,

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

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

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

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

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

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

$$\text{In summary, } n_{C2H4Oout} := 100$$

$$n_{C2H4in} = 166.667$$

$$n_{CO2out} = 133.333$$

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

$$n_{H2Oout} = 133.333$$

$$n_{O2in} = 279.848$$

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

$$n_{O2out} = 29.848$$

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:

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

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

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

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

$$C_{pO_2}(T) := 0.0291 + 1.158 \cdot 10^{-5} \cdot T - 0.6076 \cdot 10^{-8} \cdot T^2 + 1.311 \cdot 10^{-12} \cdot T^3$$

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

Cool feed down from 200 to 25:

$$dh_1 := \int_{200}^{25} n_{O2in} \cdot C_{pO_2}(T) dT \quad dh_1 = -1.485 \cdot 10^3$$

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

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

React:

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

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

Heat products to 600:

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

$$dh_7 := \int_{25}^{600} n_{O2out} \cdot C_{pO_2}(T) dT \quad dh_7 = 549.747$$

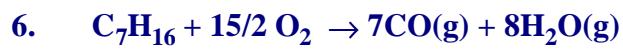
$$dh_8 := \int_{25}^{600} n_{N2out} \cdot C_{pN2}(T) dT \quad dh_8 = 1.831 \cdot 10^4$$

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

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

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

$$Q = -8.243 \cdot 10^4 \quad \text{kJ/hr}$$



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

$$\Delta H_r = -2.484 \cdot 10^3 \quad \text{kJ/mol}$$

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

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

$$\Delta H_r = -2.484 \cdot 10^3 \quad \text{kJ/mol}$$