

JQ.2.34.Soln

October 6, 2014

(2.34) Polyacrylonitrile (C_3H_3N) burns to form vapor, carbon dioxide and nitrogen. The heat of formation of the polyacrylonitrile is $15.85 \text{ kcal}/(\text{g mol})$. Use data from Tables 2.1 and 2.2. Use specific heat values at 1000K .

- (a) Write the balanced chemical equation for the stoichiometric combustion in oxygen.
- (b) Determine the heat of combustion of the polyacrylonitrile.
- (c) write the balanced chemical equation for the stoichiometric combustion in air.
- (d) Determine the adiabatic flame temperature if the fuel burns stoichiometrically in air.

Setup

Recall that a 1 gram-mol is the same as 1 mole. There is a typo $1\text{cal} = 4.18J$ and not $4.18kJ$.

You've done all these steps in previous problems. For part (a):

balance the chemical reaction using elemental balances:



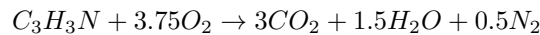
Find the stoichiometric coefficients a, b, & d.

$$C : 3 = b; \quad H : 3 = 2d; \quad N : 1 = 2f; \quad O : 2a = 2b + d$$

In [11]: `b=3.; d=3./2.; a=(2.*b+d)/2.; f=1./2.; a`

Out[11]: 3.75

We find that:



- b) Use equation 2.25 to express the heat of combustion in terms of the heats of formation

$$\Delta \tilde{h}_c = \left(\sum_i \nu_i \Delta \tilde{h}_{f,i}^o \right)_{React} - \left(\sum_j \nu_j \Delta \tilde{h}_{f,j}^o \right)_{Prod}$$

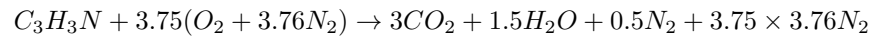
$$n_{C_3H_3N} = 1.; n_{CO_2} = 3.; n_{H_2O} = 1.5.; \Delta h_{f,CO_2}^o = -393.5 \text{ kJ}/\tilde{m}; \Delta h_{f,H_2O_{lower}}^o = -241.8 \text{ kJ}/\tilde{m}; \Delta h_{f,C_3H_3N} = 15.85 \times 4.2 \text{ kJ}/\tilde{m}$$

In [12]: `n_C3H3N=1.; n_CO2=3.; n_H2O=1.5; hfC3H3N= 15.85*4.2; hfCO2=-393.5; hfH2O_lower= -241.8;`

In [13]: `Dhcmol=hfC3H3N - (n_CO2*hfCO2 + n_H2O*hfH2O_lower); Dhcmol`

Out[13]: 1609.77

- c) It is a minor change to part (b) to find the balanced reaction in air:



d) Assume that the reactants are at $25^\circ C$.

$$T_P = 25 + \frac{m_F}{m_T} \frac{\Delta h_c}{\bar{c}} = 25 + Y_F \frac{\Delta h_c}{\bar{c}}$$

In [14]: Dhc_mole_F=1609.77; MW_F= 3*12+3+14; Dhc_mass_F= Dhc_mole_F/MW_F;

In [15]: c_mix=32.7/28. ; Y_F= 1.*MW_F/(1.*MW_F+3.75*4.76*28.8);Y_F

Out[15]: 0.09346124003667915

In [16]: T_P=25. + Y_F*Dhc_mass_F*1000./c_mix ; T_P

Out[16]: 2455.6911375383183

We find that the adiabatic flame temperature is $2455^\circ C$.