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 kcal/(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 stocihiometric combustion in oxygen.

(b) Determine the heat of combustion of the polyacrylonitrile.

(c) write the balanced chemical equation for the stocihiometric combustion in air.

(d) Determine the adiabatic flame temperature if the fuel burns stocihiometrically in in air.

Setup
Recall that a 1 gram-mol is the same as 1 mole. There is a typo $1cal = 4.18J$ and not $4.18kJ$.
You've done all these steps in previous problems. For part (a):
balance the chemical reaction using elemental balances:

$$C_3H_3N + aO_2 \rightarrow bCO_2 + dH_2O + fN2$$

Find the stoichiometric coefficients a, b,& d.
$C : 3 = b$; $H : 3 = 2d$; $N : 1 = 2f$; $O : 2a = 2b + d$

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In [11]: b=3.; d=3./2.; a=(2.*b+d)/2.; f=1./2.; a
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Out[11]: 3.75
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We find that:

$$C_3H_3N + 3.75O_2 \rightarrow 3CO_2 + 1.5H_2O + 0.5N_2$$

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

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

$n_{C3H3N} = 1.; n_{CO2} = 3.; n_{H2O} = 1.5.; \Delta h^o_{f,CO2} = -393.5kJ/\tilde{m}; \Delta h_{f,H2O_{lower}} = -241.8kJ/\tilde{m}; \Delta h_{f,C3H3N} = 15.85 \times 4.2kJ/\tilde{m}$

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In [12]: n_C3H3N=1.; n_CO2=3.; n_H2O=1.5; hfC3H3N= 15.85*4.2; hfCO2=-393.5; hfH2O_lower= -241.8;
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In [13]: Dhcmol=hfC3H3N - (n_CO2*hfCO2 + n_H2O*hfH2O_lower); Dhcmol
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Out[13]: 1609.77
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c) It is a minor change to part (b) to find the balanced rection in air:

$$C_3H_3N + 3.75(O_2 + 3.76N_2) \rightarrow 3CO_2 + 1.5H_2O + 0.5N_2 + 3.75 \times 3.76N_2$$

d) Assume that the reactants are at 25^oC.

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

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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
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We find that the adiabatic flame temperature is 2455^oC.