

JQ.2.18.soln

September 19, 2014

(2.18) Compute the heat of combustion per gram mole of acetonitrile.

Acetonitrile (C_2H_3N) burns to form hydrogen cyanide (HCN), carbon dioxide, and water vapor. Data for heat of formation are provided.

Note that gram-mole is no longer a commonly used term that refers to either the moles or a substance or on molecular weight basis. One gram mole is the molecular weight.

Table 1: Heat of formation

Species	$kcal/gmol$
HCN	32.3
C_2H_3N	21.0
H_2O	-57.8
CO_2	-94.1
O_2	0.0

This problem is similar to previous problems and introduces you to the term “gram-mole”.

Step 1: Balance the chemical reaction using elemental balances:



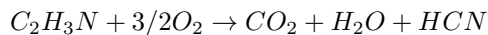
Find the stoichiometric coefficients a, b, & d.

$$N: 1 = f$$

$$C: 2 = b + f \text{ or } b = 1$$

$$H: 3 = 2d + f \text{ or } d = 1$$

$$O: 2a = 2b + d \text{ or } a = 3/2$$



Step 2: Use equation 2.25 to express the heat of combustion in terms of the heats of formation

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

In [3]: `n_C2H3N=1.; n_CO2=1.; n_H2O=1.; n_HCN=1.; hfC2H3N=21.; hfCO2=-94.1; hfH2O_lower= -57.8; hfHCN=32.3;`

In [4]: `Dhcmol=hfC2H3N - (n_CO2*hfCO2 + n_H2O*hfH2O_lower + n_HCN*hfHCN); Dhcmol`

Out[4]: 140.7

The molar heat of combustion for acetonitrile is $141 kcal/mole$. We divide by the molecular weight to get the heat of combustion on a mass basis. We divide by the mass of oxygen to get this on a oxygen basis.