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:

$$C_2H_3N + aO_2 \rightarrow bCO_2 + dH_2O + fHCN$$

Find the stoichiometric coefficients a, b,& d.

N: $1 = f$

C: $2 = b + f$ or $b = 1$

H: $3 = 2d + f$ or $d = 1$

O: $2a = 2b + d$ or $a = 3/2$

$$C_2H_3N + 3/2O_2 \rightarrow CO_2 + H_2O + HCN$$

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

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

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