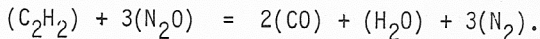


Example 1.E

The combustion of acetylene fuel with nitrous oxide as oxidant at 25°C (298 K) is widely performed in flame emission spectrophotometry. Calculate the maximum temperature attained if the best mixture corresponds to the reaction



Assume that water is undissociated.

Given: $\Delta H_{298}^0, (C_2H_2) = 54.23 \text{ kcal/mole } (226.90 \text{ kJ/mol}).$

$$\Delta H_{298}^0, (N_2O) = 19.70 \text{ kcal/mole } (82.42 \text{ kJ/mol}).$$

$$\Delta H_{298}^0, (CO) = -26.42 \text{ kcal/mole } (-110.54 \text{ kJ/mol}).$$

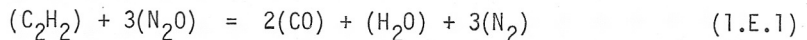
$$\Delta H_{298}^0, (H_2O) = -57.80 \text{ kcal/mole } (-241.84 \text{ kJ/mol}).$$

$$C_{P,(CO)} = 6.8 + 1.0 \times 10^{-3} T - 0.11 \times 10^5 T^{-2} \text{ cal/deg/mole} \\ (28.45 + 4.184 \times 10^{-3} T - 0.46 \times 10^5 T^{-2} \text{ J/K/mol}).$$

$$C_{P,(H_2O)} = 7.17 + 2.56 \times 10^{-3} T + 0.08 \times 10^5 T^{-2} \text{ cal/deg/mole} \\ (30.0 + 10.71 \times 10^{-3} T + 0.33 \times 10^5 T^{-2} \text{ J/K/mol}).$$

$$C_{P,(N_2)} = 6.5 + 1.0 \times 10^{-3} T \text{ cal/deg/mole} \\ (27.20 + 4.184 \times 10^{-3} T \text{ J/K/mol}).$$

Solution: The first step is to calculate the standard enthalpy change of the reaction



at 25°C. Thus, we have

$$\begin{aligned} \Delta H^0_{298,(1.E.1)} &= 2\Delta H^0_{298,(CO)} + \Delta H^0_{298,(H_2O)} - \Delta H^0_{298,(C_2H_2)} \\ &\quad - 3\Delta H^0_{298,(N_2O)} \\ &= (2 \times -26.42) + (-57.80) - (54.23) - (3 \times 19.70) \\ &= -223.97 \text{ kcal.} \end{aligned}$$

In other words, 223.97 kcal of heat is evolved during the reaction (1.E.1), which is used to heat up 2 moles of CO, 1 mole of H₂O and 3 moles of N₂ from 25°C to the final maximum temperature, say T_m. Applying Eq. (1.21), we have

$$\text{Heat evolved} = \int_{298}^{T_m} \Sigma C_{P,\text{product}} dT,$$

$$\text{or} \quad 223970 = \int_{298}^{T_m} [2C_{P,(CO)} + C_{P,(H_2O)} + 3C_{P,(N_2)}] dT$$

$$\begin{aligned}
&= \int_{298}^{T_m} \left[(13.6 + 2.0 \times 10^{-3}T - 0.22 \times 10^5 T^{-2}) + (7.17 + 2.56 \times 10^{-3}T + 0.08 \times 10^5 T^{-2}) + (19.5 + 3.0 \times 10^{-3}T) \right] dT \\
&= \int_{298}^{T_m} \left[40.27 + 7.56 \times 10^{-3}T - 0.14 \times 10^5 T^{-2} \right] dT \\
&= \left[40.27 T + 3.78 \times 10^{-3} T^2 + 0.14 \times 10^5 T^{-1} \right]_{298}^{T_m} \\
&= 40.27 (T_m - 298) + 3.78 \times 10^{-3} (T_m^2 - 298^2) + 0.14 \times 10^5 \left(\frac{1}{T_m} - \frac{1}{298} \right) \\
&= 3.78 \times 10^{-3} T_m^2 + 40.27 T_m + 0.14 \times 10^5 T_m^{-1} - 12383.
\end{aligned}$$

Neglecting the T_m^{-1} term, we have

$$223970 = 3.78 \times 10^{-3} T_m^2 + 40.27 T_m - 12383,$$

$$\text{or } 3.78 \times 10^{-3} T_m^2 + 40.27 T_m - 236353 = 0.$$

On solving the above equation in T_m and neglecting the negative value, it follows

$$T_m = 4207 \text{ K},$$

$$\begin{aligned}
\text{or } T_m &= (4207 - 273)^\circ\text{C} \\
&= 3934^\circ\text{C}.
\end{aligned}$$

Thus, the maximum temperature attained is 3934 $^\circ\text{C}$.