AFCoKaRE Practice Problem 3.3 Solution

Purpose: This problem allows you to practice calculating equilibrium constants, calculating equilibrium composition and solving sets of algebraic equations.

Problem Statement: If air (78% N_2, 22% O_2) reacts at 600 °C and atmospheric pressure and reactions (1) through (3) reach equilibrium, what will the mole percentages of N_2O, NO and NO_2 equal? Heat capacity expressions (cal mol^{-1} K^{-1}) for the reagents are given in equations (4) through (8); the standard heats of formation at 298 K of N_2O, NO and NO_2 are 19.49, 21.6 and 8.09 kcal mol^{-1}, respectively; their standard Gibbs free energies of formation at 298 K are 24.77, 20.72 and 12.42 kcal mol^{-1}, respectively.

$$N_2 + O_2 \rightarrow 2\ NO \tag{1}$$

$$2\ N_2 + O_2 \rightarrow 2\ N_2O \tag{2}$$

$$N_2 + 2\ O_2 \rightarrow 2\ NO_2 \tag{3}$$

$$\hat{C}_{p,N_2} = 7.440 - 3.24\times10^{-3}T + 6.4\times10^{-6}T^2 - 2.79\times10^{-9}T^3 \tag{4}$$

$$\hat{C}_{p,O_2} = 6.713 - 8.79\times10^{-3}T + 4.17\times10^{-6}T^2 - 2.544\times10^{-9}T^3 \tag{5}$$

$$\hat{C}_{p,NO} = 7.009 - 2.24\times10^{-3}T + 2.328\times10^{-6}T^2 - 1.0\times10^{-9}T^3 \tag{6}$$

$$\hat{C}_{p,N_2O} = 5.164 + 1.739\times10^{-2}T - 1.38\times10^{-5}T^2 + 4.371\times10^{-9}T^3 \tag{7}$$

$$\hat{C}_{p,NO_2} = 5.788 + 1.155\times10^{-2}T - 4.97\times10^{-6}T^2 + 7.0\times10^{-11}T^3 \tag{8}$$