The total number of moles is

$$n = 1 - \xi + 1 - \frac{\xi}{2} + 1 + \xi = 3 - \frac{\xi}{2},$$

and the corresponding mole fractions are

$$y_{\mathrm{NO}} = \frac{1-\xi}{3-\xi/2}, \quad y_{\mathrm{O}_2} = \frac{1-\xi/2}{3-\xi/2}, \quad y_{\mathrm{NO}_2} = \frac{1+\xi}{3-\xi/2}.$$

Treating all species in the ideal-gas state, the equilibrium constant for the reaction is

$$K_{1473} = \frac{y_{\mathrm{NO}_2}}{y_{\mathrm{NO}}\, y_{\mathrm{O}_2}^{1/2}} \cdot \left(\frac{P^\circ}{P}\right)^{1/2}.$$

Substituting the expressions for the mole fractions, this equation becomes

$$K_{1473}\left(\frac{P}{P^\circ}\right)^{1/2} = \frac{(1+\xi)(3-\xi/2)^{1/2}}{(1-\xi)(1-\xi/2)^{1/2}}. \tag{14.38}$$

The only unknown here is the extent of reaction. Because of the nonlinear nature of this equation, a trial-and-error method will be needed. Using $K_{1473} = 0.0118575$, $P = 3$ bar, $P^\circ = 1$ bar and solving for ξ we find

$$\xi = -0.9735.$$

By back substitution in the stoichiometric table we obtain the mole fractions at equilibrium:

$$y_{\mathrm{NO}} = 0.566, \quad y_{\mathrm{O}_2} = 0.426, \quad y_{\mathrm{NO}_2} = 0.00759.$$

The negative sign indicates that the reaction proceeds from ~~left to right~~.
right to left

Comments The stoichiometry of the reaction affects the value of the equilibrium constant and of the extent of reaction but not the final compositions. You should be able to confirm this by repeating these calculations using the stoichiometry of Example 14.13.

Example 14.15: Effect of Pressure
Repeat the calculation of Example 14.14 at 0.01 bar.

Solution Following the steps of Example 14.14 we find

$$\begin{aligned} \xi &= -0.9984, \\ y_{\mathrm{NO}} &= 0.571, \\ y_{\mathrm{O}_2} &= 0.428, \\ y_{\mathrm{NO}_2} &= 0.000443. \end{aligned}$$