Equlibrium Calculations Problem Set

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The equlibrium for the following chemical reaction is very temperature dependent.
2 NO2 <--> N2O4

1.Write the equlibrium expression for this reaction.

$$K=\frac{N2O4}{(NO2)\ 2}$$

2.Calculate the equlibrium constant given the initial equlibrium conditions at 320 K where:

$$P_{NO2} := 0.10\cdot atm$$

$$P_{N2O4} := 0.018\cdot atm$$

$$K_p := \frac{P_{N2O4}}{{P_{NO2}}^2}$$

$$K_p = 1.8\ atm^{-1}$$

3.Given the following initial conditions, predict the direction of the reaction.

a. $P_{NO2} := 0.10 \cdot atm$

$P_{N2O4} := 0.10 \cdot atm$

$Q_p := \frac{P_{N2O4}}{P_{NO2}^2}$

$Q_p = 10 \circ atm^{-1}$ $K_p = 1.8 \circ atm^{-1}$

If Q>K, reverse reaction favored
If Q<K, forward reaction favored

b. $P_{NO2} := 0.010 \cdot atm$

$P_{N2O4} := 0.010 \cdot atm$

$Q_p := \frac{P_{N2O4}}{P_{NO2}^2}$

$Q_p = 100 \circ atm^{-1}$ $K_p = 1.8 \circ atm^{-1}$

If Q>K, reverse reaction favored
If Q<K, forward reaction favored

c. $P_{NO2} := 1.0 \cdot atm$

$P_{N2O4} := 2.0 \cdot atm$

$Q_p := \frac{P_{N2O4}}{P_{NO2}^2}$

$Q_p = 2 \circ atm^{-1}$ $K_p = 1.8 \circ atm^{-1}$

If Q>K, reverse reaction favored
If Q<K, forward reaction favored

d. $P_{NO2} := 2.0 \cdot atm$

$P_{N2O4} := 7.0 \cdot atm$

$Q_p := \frac{P_{N2O4}}{P_{NO2}^2}$

$Q_p = 1.75 \circ atm^{-1}$ $K_p = 1.8 \circ atm^{-1}$

If Q>K, reverse reaction favored
If Q<K, forward reaction favored

e. $P_{NO2} := 0.01 \cdot atm$

$P_{N2O4} := 1.8 \cdot 10^{-4} \cdot atm$

$Q_p := \frac{P_{N2O4}}{P_{NO2}^{2}}$

$Q_p = 1.8 \circ atm^{-1}$ $K_p = 1.8 \circ atm^{-1}$

If Q>K, reverse reaction favored
If Q<K, forward reaction favored

f. $P_{NO2} := 0.5 \cdot atm$

$P_{N2O4} := 0.5 \cdot atm$

$Q_p := \frac{P_{N2O4}}{P_{NO2}^{2}}$

$Q_p = 2 \circ atm^{-1}$ $K_p = 1.8 \circ atm^{-1}$

If Q>K, reverse reaction favored
If Q<K, forward reaction favored

4.Given the initial, non-equlibrium, conditions. Calculate the equlibrium pressure of NO2 and N2O4.

a. Initial Conditions:

$$P_{NO2\_initial} := 0.20 \cdot atm$$

$$P_{N2O4\_initial} := 0.00 \cdot atm$$

Change

$$\Delta NO2 = -2 \cdot X$$

From balanced chemical reaction, NO2 goes down by 2X and N2O4 goes up by X.

$$\Delta N2O4 = X$$

Final

$$P_{NO2\_final} = P_{NO2\_initial} - 2 \cdot X$$

$$P_{N2O4\_fianl} = P_{N2O4\_initial} + X$$

Substititute into equlibrium expression:

$$K = \frac{P_{N2O4\_final}}{{P_{NO2\_final}}^2}$$

$$K = \frac{P_{N2O4\_initial} + X}{\left(P_{NO2\_initial} - 2 \cdot X\right)^2}$$

Substitute in values and solve for X:

$$1.8 \cdot atm^{-1} = \frac{X}{(0.20 \cdot atm - 2 \cdot X)^2}$$

$$X := \begin{bmatrix} .30623413613605701002 \cdot atm \\ .03265475275283187886 \cdot atm \end{bmatrix}$$

These are the two roots for X, either could be the correct answer.

Solve for the final pressures:

$$P_{NO2\_final} := P_{NO2\_initial} - 2 \cdot X \qquad P_{NO2\_final} = \begin{bmatrix} -0.412 \\ 0.135 \end{bmatrix} \cdot atm$$

$$P_{N2O4\_final} := P_{N2O4\_initial} + X \qquad P_{N2O4\_final} = \begin{bmatrix} 0.306 \\ 0.033 \end{bmatrix} \cdot atm$$

Only one of the data sets is possible, the first gives a negative pressure for NO2, this is not possible, so in this problem the second root is the one that we need to use.

b. Initial Conditions:

$$P_{NO2\_initial} := 0.00 \cdot atm$$

$$P_{N2O4\_initial} := 0.20 \cdot atm$$

Substititute into equlibrium expression:

$$1.8 \cdot atm^{-1} = \frac{0.20\ atm + X}{(0.00 \cdot atm - 2 \cdot X)^2}$$

$$X := \begin{bmatrix} .25 \cdot atm \\ -.11111111111111111111 \cdot atm \end{bmatrix}$$

These are the two roots for X, either could be the correct answer.

Solve for the final pressures:

$$P_{NO2\_final} := P_{NO2\_initial} - 2 \cdot X \qquad P_{NO2\_final} = \begin{bmatrix} -0.5 \\ 0.222 \end{bmatrix} \cdot atm$$

$$P_{N2O4\_final} := P_{N2O4\_initial} + X \qquad P_{N2O4\_final} = \begin{bmatrix} 0.45 \\ 0.089 \end{bmatrix} \cdot atm$$

Only one of the data sets is possible, the first gives a negative pressure for NO2, this is not possible, so in this problem the second root is the one that we need to use.

c. Initial Conditions:

$$P_{NO2\_initial} := 0.20 \cdot atm$$

$$P_{N2O4\_initial} := 0.20 \cdot atm$$

Substititute into equlibrium expression:

$$1.8 \cdot atm^{-1} = \frac{0.20\ atm + X}{(0.20 \cdot atm - 2 \cdot X)^2}$$

$$X := \begin{bmatrix} .38505798189250032957 \cdot atm \\ -.04616909300361144069 \cdot atm \end{bmatrix}$$

These are the two roots for X, either could be the correct answer.

Solve for the final pressures:

$$P_{NO2\_final} := P_{NO2\_initial} - 2 \cdot X \qquad P_{NO2\_final} = \begin{bmatrix} -0.57 \\ 0.292 \end{bmatrix} \circ atm$$

$$P_{N2O4\_final} := P_{N2O4\_initial} + X \qquad P_{N2O4\_final} = \begin{bmatrix} 0.585 \\ 0.154 \end{bmatrix} \circ atm$$

Only one of the data sets is possible, the first gives a negative pressure for NO2, this is not possible, so in this problem the second root is the one that we need to use.