Reactions such as the one in the previous example involve the dissociation of a molecule. Such reactions can be easily described in terms of the fraction of reactant molecules that actually dissociate to achieve equilibrium in a sample. This fraction is called the **degree of dissociation**. For the reaction in the previous example

\[ A(g) \rightleftharpoons 2 B(g) \]

the degree of dissociation can be used to fill out an ICE table. If the reaction is started with \( n \) moles of \( A \), and \( \alpha \) is the fraction of \( A \) molecules that dissociate, the ICE table will look as follows.

<table>
<thead>
<tr>
<th></th>
<th>( A )</th>
<th>( 2 , B )</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Initial</strong></td>
<td>( n )</td>
<td>0</td>
</tr>
<tr>
<td><strong>Change</strong></td>
<td>(-\alpha n)</td>
<td>(+2n\alpha)</td>
</tr>
<tr>
<td><strong>Equilibrium</strong></td>
<td>( n(1-\alpha) )</td>
<td>( 2n\alpha )</td>
</tr>
</tbody>
</table>

The mole fractions of \( A \) and \( B \) can then be expressed by

\[
\begin{align*}
\chi_A &= \frac{n(1-\alpha)}{n(1-\alpha)+2n\alpha} \\
&= \frac{1-\alpha}{1+\alpha} \\
\chi_B &= \frac{2\alpha}{1+\alpha}
\end{align*}
\]

Based on these mole fractions

\[
\begin{align*}
K_x &= \left( \frac{2\alpha}{1+\alpha} \right)^2 \left( \frac{1-\alpha}{1+\alpha} \right) \\
&= \frac{4\alpha^2}{1-\alpha^2}
\end{align*}
\]

And so \( K_p \), which can be expressed as

\[
K_p = K_x (p_{tot})^{\sum \nu_i}
\]

is given by

\[
K_p = \frac{4\alpha^2}{1-\alpha^2} (p_{tot})
\]

Example \( \PageIndex{1} \)

Based on the values given below, find the equilibrium constant at 25 °C and degree of dissociation for a system that is at a total pressure of 1.00 atm for the reaction

\[ N_2O_4(g) \rightleftharpoons 2 \, NO_2(g) \]

<table>
<thead>
<tr>
<th>( \Delta G_f^o ) (kJ/mol)</th>
<th>( N_2O_4(g) )</th>
<th>( NO_2(g) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>99.8</td>
<td>(nonumber)</td>
<td>51.3</td>
</tr>
</tbody>
</table>

Solution
First, the value of $K_p$ can be determined from $\Delta G_{rxn}^o$ via an application of Hess’ Law.

\[
\begin{align*}
\Delta G_{rxn}^o &= 2 \left( 51.3 \, kJ/mol \right) - 99.8 \,kJ/mol &= 2.8 \, kJ/mol
\end{align*}
\]

So, using the relationship between thermodynamics and equilibria

\[
\begin{align*}
\Delta G_f^o &= -RT \ln K_p \\
2800 \, kJ/mol &= -(8.314 \, J/(mol\,K) \left( 298 \,K \right) \ln K_p \\
K_p &= 0.323 \, atm
\end{align*}
\]

The degree of dissociation can then be calculated from the ICE tables at the top of the page for the dissociation of $N_2O_4(g)$:

\[
\begin{align*}
K_p &= \dfrac{4 \alpha^2}{1-\alpha^2} (p_{tot}) \\
0.323 \, atm &= \dfrac{4 \alpha^2}{1-\alpha^2} (1.00 \, atm)
\end{align*}
\]

Solving for $\alpha$,

\[
\alpha = 0.273 \nonumber
\]

Note: since $\alpha$ represents the fraction of $N_2O_4$ molecules dissociated, it must be a positive number between 0 and 1.

Example $(PageIndex{2})$

Consider the gas-phase reaction

\[
A + 2B \rightleftharpoons 2C
\]

A reaction vessel is initially filled with 1.00 mol of A and 2.00 mol of B. At equilibrium, the vessel contains 0.60 mol C and a total pressure of 0.890 atm at 1350 K.

1. How many mol of A and B are present at equilibrium?
2. What is the mole fraction of A, B, and C at equilibrium?
3. Find values for $(K_x)$, $(K_p)$, and $(\Delta G_{rxn}^o)$.

Solution:

Let’s build an ICE table!

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>2 B</th>
<th>2 C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>1.00 mol</td>
<td>2.00 mol</td>
<td>0</td>
</tr>
<tr>
<td>Change</td>
<td>-x</td>
<td>-2x</td>
<td>+2x</td>
</tr>
<tr>
<td>Equilibrium</td>
<td>1.00 mol - x</td>
<td>2.00 mol - 2x</td>
<td>2x = 0.60 mol</td>
</tr>
</tbody>
</table>

From the equilibrium measurement of the number of moles of C, $x = 0.30$ mol. So at equilibrium,
The total number of moles at equilibrium is 2.70 mol. From these data, the mole fractions can be determined.

\[
\begin{align*}
\chi_A &= \frac{0.70\,\text{mol}}{2.70\,\text{mol}} = 0.259 \\
\chi_B &= \frac{1.40\,\text{mol}}{2.70\,\text{mol}} = 0.519 \\
\chi_C &= \frac{0.60\,\text{mol}}{2.70\,\text{mol}} = 0.222
\end{align*}
\]

So \(K_x\) is given by

\[
K_x = \frac{(0.222)^2}{(0.259)(0.519)^2} = 0.7064
\]

And \(K_p\) is given by Equation \ref{oddEq}, so

\[
K_p = 0.7604(0.890 \,\text{atm})^{-1} = 0.792,\,\text{atm}^{-1}
\]

The thermodynamic equilibrium constant is unitless, of course, since the pressures are all divided by 1 atm. So the actual value of \(K_p\) is 0.794. This value can be used to calculate \(\Delta G_{\text{rxn}}^o\) using

\[
\Delta G_{\text{rxn}}^o = -RT \ln K_p
\]

so

\[
\begin{align*}
\Delta G_{\text{rxn}}^o &= - (8.314 \,\text{J/(mol\,K)})( 1350 \,\text{K}) \ln (0.792) \\
&= 2590 \,\text{J/mol}
\end{align*}
\]

Contributors

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