Chapter 11 Homework Solution Tips

11.1
This is a reaction extent problem.
Note: for gases: volume percent = mole percent = pressure percent
Get K from $\Delta G^\circ$

11.2
This is a reaction extent problem.
Note: for gases: volume percent = mole percent = pressure percent
Get K from $\Delta G^\circ$
Once the moles of SO$_3$ formed is determined from the reaction extent calc, multiply by the $\Delta H^\circ_R$.

11.3
The overall reaction is
$$2H_2 + CO_2 = 2H_2O + 2CO$$
This is composed of the two reactions
$$2H_2 + O_2 = 2H_2O$$
$$2CO + O_2 = 2CO_2$$
Since the pressure of O$_2$ is specified and the same in both reactions, the K's for the two reactions give two equations relating the four unknowns (the moles of each gas). Since all the H$_2$O and CO come from the overall reaction (the amount of O$_2$ formed is negligible), the moles of H$_2$O and CO are equal. This is a third equation relating the four unknowns. There are infinite multiples of H$_2$ and CO$_2$ that give the same equilibrium pressures. We need only one to fix a ratio of initial H$_2$/CO$_2$ so simply assume a basis of calculation, say 100 moles of either H$_2$ or CO$_2$.

*Note an important engineering problem solving tip:*
Any problem involving ratios, rates, fractions, proportions, or percentages always requires your setting a BASIS OF CALCULATION.
The assumed basis value has makes difference to the outcome.

11.4
The pressure of Br is that of Li (stoichiometry) and the pressure of LiBr is still essentially unity. So substitute pressures into K and find K. Then find $\Delta G^\circ = RT \ln K = A + BT$ and solve for T since $\Delta G^\circ = A + BT$. 
11.5

\[ 2\text{SO}_3 = 2\text{SO}_2 + \text{O}_2 \quad \text{K} \]

Set a basis of calculation of 1 mole of \text{SO}_3 initially.

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The assumed basis value has makes difference to the outcome.

Let \( x \) = moles of \text{O}_2 produced.

**Mole Balance**

<table>
<thead>
<tr>
<th>Species</th>
<th>Initial</th>
<th>Final (Equil)</th>
<th>( P_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>\text{SO}_3</td>
<td>1</td>
<td>1-2x</td>
<td>\frac{[(1-2x)/(1+x)]P_T}{P_T}</td>
</tr>
<tr>
<td>\text{SO}_2</td>
<td>0</td>
<td>2x</td>
<td>\frac{[2x/(1+x)]P_T}{P_T}</td>
</tr>
<tr>
<td>\text{O}_2</td>
<td>0</td>
<td>x</td>
<td>\frac{[x/(1+x)]P_T}{P_T}</td>
</tr>
<tr>
<td>Total</td>
<td>1</td>
<td>1+x</td>
<td>( P_T )</td>
</tr>
</tbody>
</table>

\[
K = \frac{P_{\text{SO}_2}^2 P_{\text{O}_2}}{P_{\text{SO}_3}^2} = \frac{\left( \frac{2x}{1+x} \right)^2}{\left( \frac{1-2x}{1+x} \right)^2} P_{\text{O}_2} \quad (1)
\]

\[
K = \left( \frac{2x}{1-2x} \right)^2 P_{\text{O}_2} \quad (2)
\]

\[
P_{\text{O}_2} = \frac{x}{1+x} P_T \quad (3)
\]

\( P_{\text{O}_2} = 0.05 \text{ atm} \) is given for the given \( T \) of 1000 K and the unknown requested \( T \).

**Mathematical considerations;**

*At \( T = 1000 \text{ K} \)*

The unknowns are \( x \) and \( P_T \). Use Equations (2) and (3) to solve.

*At \( P_T = 1 \text{ atm} \)*

The unknowns are \( x \) and \( K \). Use Equations (2) and (3) to solve.

Once \( K \) is known, solve \( \Delta G^o = -RT \ln K = A + BT \) for \( T \).

Do not get mathematical complexity confused with the thermodynamic simplicity.
11.6
Solve for K. Sub into K. Assume PN2 = 1 atm. Solve for PN.

11.7
(3/2)H2 + (1/2)N2 = NH3  
K (known from ΔG° = A + BT)

Set a basis of calculation of 1 mole of NH3 initially.

Note an important engineering problem solving tip:
Any problem involving ratios, rates, fractions, proportions, or percentages always requires your setting a BASIS OF CALCULATION.

The assumed basis value has makes difference to the outcome.

Let x = moles of N2 produced from the decomposition of NH3

Mole Balance

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<th>Pi</th>
</tr>
</thead>
<tbody>
<tr>
<td>NH3</td>
<td>1</td>
<td>1 - 2x</td>
<td>[(1-2x)/(1+2x)]P_T</td>
</tr>
<tr>
<td>H2</td>
<td>0</td>
<td>3x</td>
<td>[3x/(1+2x)]P_T</td>
</tr>
<tr>
<td>N2</td>
<td>0</td>
<td>x</td>
<td>[x/(1+2x)]P_T</td>
</tr>
<tr>
<td>Total</td>
<td>1</td>
<td>1 + 2x</td>
<td>P_T</td>
</tr>
</tbody>
</table>

The mole fraction of N2 = 0.2 = x/(1 + 2x). Therefore, x is easily determined.
The value of P_T is then easily determined from

\[
K = \frac{P_{NH3}^{\frac{3}{2}}P_{H2}^{\frac{1}{2}}}{P_{N2}^{\frac{3}{2}}P_{H2}^{\frac{1}{2}}} = \frac{\left(\frac{1-2x}{1+2x}\right)P_T^{\frac{3}{2}}}{\left(\frac{3x}{1+2x}\right)P_T^{\frac{1}{2}}} \left(\frac{Y_{N2}}{P_T}\right) \frac{1}{\left(\frac{Y_{N2}}{P_T}\right)^{\frac{1}{2}}}
\]

\[Y_{N2} = \text{N}_2 \text{ mole fraction} = 0.2\]

\[
P_T = \frac{(1 - 2x)(1 + 2x)^{\frac{1}{2}}}{0.2K (3x)^{\frac{3}{2}}}
\]

Do not get mathematical complexity confused with the thermodynamic simplicity.

11.8
As with problems 11.5 and 11.7, setup a reaction extent solution. Once the partial pressures are substituted into the K, the only unknowns are the reaction extent, x, and the initial moles of PCl3 (assuming the basis of 1 mole of PCl5 initially). The two equations to solve these are the K = --- expression and the partial pressure of Cl2 expression containing only x and the known P_T.

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The assumed basis value has makes difference to the outcome.

Do not get mathematical complexity confused with the thermodynamic simplicity.
\[
\text{H}_2 + \frac{1}{2} \text{O}_2 = \text{H}_2\text{O} \quad \text{K (known from } \Delta G^0 = A + BT)\]

Set a basis of calculation of 1 mole of \( \text{H}_2 \) initially.

Let \( 2x \) = moles of \( \text{H}_2\text{O} \) produced

### Mole Balance

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<th>Final (Equil)</th>
<th>( P_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{O}_2 )</td>
<td>0.21</td>
<td>0.21-( x )</td>
<td>((0.21-x)/(5-x))( P_T )</td>
</tr>
<tr>
<td>( \text{N}_2 )</td>
<td>0.79</td>
<td>0.79</td>
<td>etc</td>
</tr>
<tr>
<td>( \text{H}_2 )</td>
<td>4</td>
<td>4-2( x )</td>
<td></td>
</tr>
<tr>
<td>( \text{H}_2\text{O} )</td>
<td>0</td>
<td>2( x )</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>1</td>
<td>5-x</td>
<td>( P_T = 1 )</td>
</tr>
</tbody>
</table>

Substitute into \( \text{K} \) and solve for \( x \), etc. Once \( x \) is known, multiply the reaction enthalpy and entropy change per mole as written by the corresponding reaction extent.

Do not get mathematical complexity confused with the thermodynamic simplicity.