Lecture 9 – Chapter 14, review
Temperature dependence of $\Delta G$
Announcements

• CAPA #5 due today
  – CAPA help! Sun night 7:00 Schaap 3031
    Wed night 8:00 Schaap 3031

• Extra credit
  – Attend research celebration today (3-6 pm, DeVos) and
    talk to at least two students. Write up summary and
    turn in.
ΔG is really important!

We saw three key things last week that should be re-emphasized

\[ \Delta G_{rxn} = \Delta G^\circ_{rxn} + RT \ln Q \]

\[ \Delta G = \Delta H - T\Delta S \]

<table>
<thead>
<tr>
<th>( \Delta H^\circ )</th>
<th>( \Delta S^\circ )</th>
<th>( \Delta G^\circ ) (high T)</th>
<th>( \Delta G^\circ ) (low T)</th>
<th>Spontaneous</th>
</tr>
</thead>
<tbody>
<tr>
<td>–</td>
<td>+</td>
<td>–</td>
<td>–</td>
<td>All T</td>
</tr>
<tr>
<td>+</td>
<td>–</td>
<td>+</td>
<td>+</td>
<td>No T</td>
</tr>
<tr>
<td>+</td>
<td>+</td>
<td>–</td>
<td>+</td>
<td>High T (entropy driven)</td>
</tr>
<tr>
<td>–</td>
<td>–</td>
<td>+</td>
<td>–</td>
<td>Low T (enthalpy driven)</td>
</tr>
</tbody>
</table>
\[ \Delta G_{rxn} = \Delta G^\circ_{rxn} + RT \ln Q \]

- Let’s work our way through an example using copper chloride

\[ \text{FeOH}_3(s) \rightarrow \text{Fe}^{3+}(aq) + 3\text{OH}^-(aq) \]

\[ \Delta G_f^\circ(\text{FeOH}_3(s)) = -696.5 \text{ kJ/mol} \]
\[ \Delta G_f^\circ(\text{Fe}^{3+}(aq)) = -4.72 \text{ kJ/mol} \text{ (I’m making this one up)} \]
\[ \Delta G_f^\circ(\text{OH}^-(aq)) = -157.244 \text{ kJ/mol} \]

So what is \( \Delta G^\circ_{Rxn} \) for this reaction?
What is $\Delta G^\circ_{rxn}$ for dissolving iron hydroxide?

$\text{FeOH}_3(s) \rightarrow \text{Fe}^{3+}(aq) + 3\text{OH}^-(aq)$

$\Delta G_f^\circ(\text{FeOH}_3(s)) = -696.5 \text{ kJ/mol}$

$\Delta G_f^\circ(\text{Fe}^{3+}(aq)) = -4.72 \text{ kJ/mol}$

$\Delta G_f^\circ(\text{OH}^-(aq)) = -157.244 \text{ kJ/mol}$
So, the $\Delta G_{\text{rxn}}^\circ$ for dissolving iron hydroxide is 220 kJ/mol.

What about if $[\text{Fe}^{3+}] = 0.001 \text{ M}$ and $[\text{OH}^-] = 0.001 \text{ M}$?

Note that $[\text{FeOH}_3] = 1$ by definition (it is a solid)

(At room temperature)

$$
\Delta G_{\text{rxn}} = \Delta G_{\text{rxn}}^\circ + RT \ln Q
$$

(remember Q is products over reactants)

25% 1. $-2.3 \times 10^4 \text{ kJ/mol}$

25% 2. 152 kJ/mol

25% 3. 186 kJ/mol

25% 4. 289 kJ/mol
ΔG is really important!

The last two things are really the same

\[ ΔG = ΔH - TΔS \]
Why?

• This is critical because understanding when reactions occur spontaneously is critical.

• We need to know what $\Delta G$ is favorable or not.
  – Of course, this is related to enthalpy and entropy.
When is enthalpy favorable?

- 33% 1. $\Delta H < 0$
- 33% 2. $\Delta H = 0$
- 33% 3. $\Delta H > 0$
When is entropy favorable?

| 33%  | 1. $\Delta S < 0$ |
| 33%  | 2. $\Delta S = 0$ |
| 33%  | 3. $\Delta S > 0$ |
When is free energy favorable?

<table>
<thead>
<tr>
<th>33%</th>
<th>1. $\Delta G &lt; 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>33%</td>
<td>2. $\Delta G = 0$</td>
</tr>
<tr>
<td>33%</td>
<td>3. $\Delta G &gt; 0$</td>
</tr>
</tbody>
</table>
Temperature dependence

• Let’s look at some hypothetical reaction
  – $\Delta H^\circ_{Rxn}$ is $-147.6$ kJ/mol
  – $\Delta S^\circ_{Rxn}$ is $-218.1$ J/K·mol

• What is $\Delta G^\circ_{Rxn}$?

$$\Delta G = \Delta H - T\Delta S$$
If $\Delta H^\circ_{Rxn} = -147.6 \text{ kJ/mol}$
and $\Delta S^\circ_{Rxn} = -218.1 \text{ J/K/mol}$

What is $\Delta G^\circ_{Rxn}$

25% 1. $-88.1 \text{ kJ/mol}$
25% 2. $-82.6 \text{ kJ/mol}$
25% 3. 64.9 kJ/mol
25% 4. 64900 kJ/mol
If $\Delta H^\circ_{Rxn} = -147.6 \text{ kJ/mol}$
and $\Delta S^\circ_{Rxn} = -218.1 \text{ J/K} \cdot \text{mol}$

What is $\Delta G^\circ_{Rxn}$ at 10 K?
If $\Delta H^\circ_{Rxn} = -147.6 \text{ kJ/mol}$
and $\Delta S^\circ_{Rxn} = -218.1 \text{ J/K} \cdot \text{mol}$

What is $\Delta G^\circ_{Rxn}$ at 1000 K?

<table>
<thead>
<tr>
<th>Answer</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. $-365.7 \text{ kJ/mol}$</td>
<td>25%</td>
</tr>
<tr>
<td>2. 0 $\text{ kJ/mol}$</td>
<td>25%</td>
</tr>
<tr>
<td>3. 70.5 $\text{ kJ/mol}$</td>
<td>25%</td>
</tr>
<tr>
<td>4. 218.1 $\text{ kJ/mol}$</td>
<td>25%</td>
</tr>
</tbody>
</table>
ΔG is really important!

So when \( T \) is tiny, \( ΔG \) is approximately \( ΔH \)
When \( T \) is huge \( ΔG \) is similar to \( ΔS \).

\[
ΔG = ΔH - TΔS
\]
Today

• Research Celebration! (DeVos 3-6)
• CAPA #5
  – CAPA help! Sun night 7:00 Schaap 3031
     Wed night 8:00 Schaap 3031

Tuesday

• Special seminar 11:00 VDW 102

Wednesday

• Read Chapter 15
• Fall in love with kinetics