Putting it all together: relating nonstandard values of $\Delta H$ and $\Delta E$

In many problems, you will need to interconvert $\Delta H$ and $\Delta E$ and you will have to deal with nonstandard values. In any situation where you must interconvert $\Delta H$ and $\Delta E$, you should always use the standard values. In other words, your strategy map should look like this:

(heat at constant pressure) nonstandard $\Delta H$ $\ce{<->}$ standard $\Delta H$ $\ce{<->}$ standard $\Delta E$ $\ce{<->}$ nonstandard $\Delta E$ (heat at constant volume)

You can work through the above sequence either forward or backward, and you can start and end anywhere on the map. The following examples illustrate some typical problem types.

Example $\PageIndex{1}$:

Consider the following reaction:

$$\ce{2CO(g) + O2(g) -> 2CO2(g)}$$ \hspace{1cm} $\Delta E = -563.5 \text{ kJ}$

How much heat will be given off if 7.130 moles of CO reacts with excess O$_2$ in an open container at 25°C?

In an open container (constant pressure), the heat equals $\Delta H$, so we are going to need to convert $\Delta E$ into $\Delta H$. We were given the standard value of $\Delta E$, so we can start by using the equation $\Delta H = \Delta E + RT\Delta n_{\text{gases}}$ to calculate the standard value of $\Delta H$. Once we know that, we can work out the nonstandard value of $\Delta H$, which will equal the heat.

Using $\Delta H = \Delta E + RT\Delta n_{\text{gases}}$ gives us:

$$\Delta H = -563.5 \text{ kJ} + (8.314 \text{ J/mol} \times \text{K})(298.15 \text{ K})(2 \text{ mol} - 3 \text{ mol})$$

$$= -563.5 \text{ kJ} + (-2479 \text{ J})$$

$$= -563.5 \text{ kJ} + (-2.479 \text{ kJ})$$

$$= -566.0 \text{ kJ}$$

This is $\Delta H_{\text{standard}}$ for the reaction, corresponding to the reaction of 2 moles of CO with 1 mole of O$_2$. Now
we calculate the nonstandard value of \(\Delta H\) that corresponds to the reaction of 7.130 moles of CO.

\[
\frac{-566.0 \text{ kJ}}{2 \text{ mol CO}} = \frac{\Delta H_{\text{nonstandard}}}{7.130 \text{ mol CO}}
\]

Solving this equation gives \(\Delta H_{\text{nonstandard}} = -2018 \text{ kJ}\), so the reaction will give off **2018 kJ of heat**.

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**Example (PageIndex(2))**:

When 0.07563 mol of gaseous \(\text{C}_4\text{H}_{10}\) reacts with oxygen in a sealed, rigid container, 217.6 kJ of heat is given off. Calculate \(\Delta H\) for the following reaction at 25°C:

\[
\text{\ce{2C4H10(g) + 13O2(g) -> 8CO2(g) + 10H2O(l)}}
\]

First, let’s be sure that we understand what we’re trying to calculate; the problem is asking for the **standard** value of \(\Delta H\) for this reaction. In other words, we need to calculate the enthalpy change when 2 moles of \(\text{C}_4\text{H}_{10}\) burns.

Now, let’s understand the numbers we are given. We are given the amount of heat that is produced when 0.7563 moles of \(\text{C}_4\text{H}_{10}\) burns in a rigid container. The heat is given off, so \(q\) is a negative number: \(q = -217.6 \text{ kJ}\). Under these conditions, the volume is constant, so the heat equals \(\Delta E\) (not \(\Delta H\)). This is a nonstandard value, because we didn’t use 2 moles of \(\text{C}_4\text{H}_{10}\), so we can say that \(\Delta E_{\text{nonstandard}} = -217.6 \text{ kJ}\). To convert \(\Delta E\) into \(\Delta H\), we need the standard value of \(\Delta E\). Therefore, our strategy will be:

nonstandard \(\Delta E\) \(\rightarrow\) standard \(\Delta E\) \(\rightarrow\) standard \(\Delta H\)

We are now ready to start calculating. First, we convert the nonstandard value of \(\Delta E\) into the standard value:

\[
\frac{\Delta E_{\text{standard}}}{2 \text{ mol } \text{C}_4\text{H}_{10}} = \frac{-217.6 \text{ kJ}}{0.07563 \text{ mol } \text{C}_4\text{H}_{10}}
\]

Solving this equation gives \(\Delta E_{\text{standard}} = -5754.33 \text{ kJ}\)

Finally, we convert the standard value of \(\Delta E\) into the standard value of \(\Delta H\):

\[
\Delta H = \Delta E + RT\Delta n_{\text{gases}}
\]

\[
= -5754.33 \text{ kJ} + (8.314 \text{ J/mol}\times\text{K})(298.15 \text{ K})(8 \text{ mol} - 15 \text{ mol})
\]

\[
= -5754.33 \text{ kJ} + (-17352 \text{ J})
\]

\[
= -5754.33 \text{ kJ} + (-17.352 \text{ kJ})
\]
Example \(\PageIndex{3}\)):

When 1.500 g of MgS reacts with excess oxygen at constant pressure, 9.207 kJ of heat is given off. How much heat would be given off if the same amount of MgS reacted with oxygen at constant volume? Assume a temperature of 25˚C for both reactions. The chemical reaction is \(\text{MgS(s)} + 2 \text{O}_2(g) \rightarrow \text{MgSO}_4(s)\)

We are given the heat at constant pressure, which equals \(\Delta H\). This is a nonstandard value, because we did not use 1 mole of MgS. Our final answer will be a nonstandard value of \(\Delta E\), since the heat equals \(\Delta E\) when the volume is constant. Our strategy will be:

\[
\text{nonstandard } \Delta H \rightarrow \text{standard } \Delta H \rightarrow \text{standard } \Delta E \rightarrow \text{nonstandard } \Delta E
\]

To begin, we convert the nonstandard \(\Delta H\) value into the standard value. The molar mass of MgS is 56.37 g/mol, so 1.500 g equals 0.0266099 mol of MgS. Using our normal setup:

\[
\frac{\Delta H_{\text{standard}}}{1 \text{ mol MgS}} = \frac{-9.207 \text{ kJ}}{0.0266099 \text{ mol MgS}}
\]

Solving this equation gives \(\Delta H_{\text{standard}} = -345.999 \text{ kJ}\).

Next, we translate our standard \(\Delta H\) into the standard \(\Delta E\):

\[
\Delta H = \Delta E + RT\Delta n_{\text{gases}}
\]

\[-345.999 \text{ kJ} = \Delta E + (8.314 \text{ J/mol×K})(298.15 \text{ K})(0 \text{ mol} – 2 \text{ mol})
\]

Solving this equation gives \(\Delta E = -341.041 \text{ kJ}\). This is \(\Delta E_{\text{standard}}\).

Finally, we calculate \(\Delta E_{\text{nonstandard}}\) for the reaction of 0.0266099 moles of MgS, which will equal our heat.

\[
\frac{-341.041 \text{ kJ}}{1 \text{ mol MgS}} = \frac{\Delta E_{\text{nonstandard}}}{0.0266099 \text{ mol MgS}}
\]

Solving this equation gives \(\Delta E_{\text{nonstandard}} = -9.075 \text{ kJ}\). We conclude that the reaction gives off 9.075 kJ of heat at constant volume.

Example \(\PageIndex{4}\)):
For the reaction $2 \text{KClO}_3(s) \rightarrow 2 \text{KCl}(s) + 3 \text{O}_2(g)$, $\Delta H = -90 \text{kJ}$. What are $q$ and $w$ when 2 moles of solid $\text{KClO}_3$ reacts at constant pressure and 25˚C? What is $(\Delta E)$ under these conditions?

The reaction is carried out at constant pressure, so $q = \Delta H$. The problem states that we are using 2 moles of $\text{KClO}_3$, which matches the coefficient in the balanced equation, so we can use the standard value of $\Delta H$: $q = -90 \text{kJ}$.

To calculate $w$, we use the formula $w = -RT\Delta n_{\text{gases}}:
\begin{align*}
w &= -(8.314 \text{ J/mol×K})(298.15 \text{ K})(3 \text{ mol} - 0 \text{ mol}) = -7436 \text{ J} \\
\text{Converting to kilojoules (to be consistent with } q) \text{ gives } w &= -7.436 \text{ kJ}.
\end{align*}$

To calculate $(\Delta E)$, we can use our familiar relationship between $\Delta E$ and $\Delta H$. However, it is easier to use the First Law of Thermodynamics: $\Delta E = q + w$. Substituting in the values of $q$ and $w$ we just calculated gives $(\Delta E) = -97 \text{kJ}$. This reaction produces 97 kJ of energy, of which 90 kJ is released as heat and 7 kJ is used to do PV work.

Note that the PV work we just calculated is the standard value, corresponding to 2 moles of $\text{KClO}_3$ reacting. The next example shows how to deal with a situation where you have a nonstandard amount of reactant.

**Example:**

*If you want to get 2.000 kJ of PV work from the reaction in the previous example, how much $\text{KClO}_3$ should you use?*

In the previous example, we found that 7.436 kJ of PV work is done when 2 moles of $\text{KClO}_3$ reacts. The PV work is proportional to the amount of reactant (just like $\Delta E$ and $\Delta H$), so we can use the usual technique to calculate the amount of $\text{KClO}_3$ here.

$\frac{7.436 \text{kJ}}{2 \text{ mol } \text{KClO}_3} = \frac{2.000 \text{kJ}}{n_{\text{nonstandard}}}$

Solving this equation gives $n_{\text{nonstandard}} = 0.5379$ moles of $\text{KClO}_3$. 