- Free Energy and Equilibrium

Example \#2: Octane gas, $\mathrm{C}_{8} \mathrm{H}_{18}$, is used in gasoline. Use the data below to answer the following questions about the combustion of octane gas.

| Substance | $\Delta H_{f}^{0}\left(\mathrm{~kJ} \mathrm{~mol}^{-1}\right)$ | $S^{0}\left(\mathrm{~J} \mathrm{~mol}^{-1} \mathrm{~K}^{-1}\right)$ |
| :---: | :---: | :---: |
| $\mathrm{C}_{8} \mathrm{H}_{18(\mathrm{~g})}$ | -208.4 | 345.3 |
| $\mathrm{O}_{2(\mathrm{~g})}$ | 0 | 205.1 |
| $\mathrm{CO}_{2(\mathrm{~g})}$ | -393.5 | 213.7 |
| $\mathrm{H}_{2} \mathrm{O}_{(\mathrm{l})}$ | -285.8 | 188.8 |

Use the data above to answer the questions that follow. Assume all reactions take place at $25^{\circ} \mathrm{C}$.
a) Write a complete balanced chemical equation for the combustion of octane. Assume that carbon dioxide and water are the only products.

$$
2 \mathrm{C}_{8} \mathrm{H}_{18(\mathrm{~g})}+25 \mathrm{O}_{2(\mathrm{~g})} \rightarrow 16 \mathrm{CO}_{2(\mathrm{~g})}+18 \mathrm{H}_{2} \mathrm{O}_{(\mathrm{l})}
$$

b) Calculate the standard enthalpy change, $\Delta H^{0}$, for the combustion of one mole of octane gas.

$$
\Delta H_{r x n}^{0}=\Sigma \Delta H_{f}^{0} \text { (products) }-\Sigma \Delta H_{f}^{0} \text { (reactants) }
$$

$$
\Delta H_{c o m b}^{0}=\left[16\left(\frac{-393.5 \mathrm{~kJ}}{\mathrm{~mol}}\right)+18\left(\frac{-285.8 \mathrm{~kJ}}{\mathrm{~mol}}\right)\right]-\left[2\left(\frac{-208.4 \mathrm{~kJ}}{\mathrm{~mol}}\right)+25\left(\frac{0 \mathrm{~kJ}}{\mathrm{~mol}}\right)\right]=-11023.6 \frac{\mathrm{~kJ}}{\mathrm{~mol}}
$$

Typically the question wants to know the enthalpy change for one mole of octane gas: Therefore,

$$
\begin{gathered}
\Delta H_{c o m b}^{0}=-11023.6 \frac{\mathrm{~kJ}}{\mathrm{~mol}} \text { for } 2 \mathrm{moles} \text { of } \mathrm{C}_{8} \mathrm{H}_{18(\mathrm{~g})} \\
\text { For } 1 \text { mole of } \mathrm{C}_{8} \mathrm{H}_{18(\mathrm{~g})}: \frac{-11023.6 \frac{\mathrm{~kJ}}{\mathrm{~mol}}}{2}=-5511.8 \frac{\mathrm{~kJ}}{\mathrm{~mol}}
\end{gathered}
$$

c) Calculate the standard entropy change, $\Delta S^{0}$, for the combustion of one mole of octane gas.

$$
\begin{gathered}
\Delta S_{r x n}^{0}=\Sigma \Delta S^{0} \text { (products) }-\Sigma \Delta S^{0} \text { (reactants) } \\
\Delta S_{r x n}^{0}=\left[16\left(\frac{213.7 \mathrm{~J}}{\mathrm{~mol} \cdot \mathrm{~K}}\right)+18\left(\frac{188.8 \mathrm{~J}}{\mathrm{~mol} \cdot \mathrm{~K}}\right)\right] \\
-\left[2\left(\frac{345.3 \mathrm{~J}}{\mathrm{~mol} \cdot \mathrm{~K}}\right)+25\left(\frac{205.1 \mathrm{~J}}{\mathrm{~mol} \cdot \mathrm{~K}}\right)\right]=+999.5 \frac{\mathrm{~J}}{\mathrm{~mol} \cdot \mathrm{~K}} \\
\\
\text { For 1 mole of } \mathrm{C}_{8} \mathrm{H}_{18(\mathrm{~g})}: \frac{+999.5 \frac{\mathrm{~J}}{\mathrm{~mol} \cdot \mathrm{~K}}}{2}=+499.75 \frac{\mathrm{~J}}{\mathrm{~mol} \cdot \mathrm{~K}}
\end{gathered}
$$

d) Determine the value of $\Delta G^{0}$ for the reaction.

$$
\Delta G=\Delta H-T \Delta S
$$

$$
\begin{gathered}
\text { Convert }(\mathrm{J} \text { to } \mathrm{kJ}): \Delta S=\left(+499.75 \frac{\mathrm{~J}}{\mathrm{~mol} \cdot \mathrm{~K}}\right)\left(\frac{1 \mathrm{~kJ}}{1000 \mathrm{~J}}\right)=+0.49975 \frac{\mathrm{~kJ}}{\mathrm{~mol} \cdot \mathrm{~K}} \\
\Delta G=\left(-5511.8 \frac{\mathrm{~kJ}}{\mathrm{~mol}}\right)-(298 \mathrm{~K})\left(+0.49975 \frac{\mathrm{~kJ}}{\mathrm{~mol} \cdot \mathrm{~K}}\right)=-5661 \frac{\mathrm{~kJ}}{\mathrm{~mol}}
\end{gathered}
$$

