The following are common thermodynamic equations and sample problems showing a situation in which each might be used.

**Work and Transfer of Heat and Energy**

\[ q = mC_p\Delta T \]

- \( q \) is the heat in J
- \( m \) is the mass in g
- \( C_p \) is the specific heat in J/(g C)
- \( \Delta T \) is the change in temperature in Kelvin or Celsius

**Q1**

How many liters of water can 6.7 L of ethane boil? The initial temperature and pressure of the ethane and water is 0.95 bar and 25˚C.

**Solution**

First we must find the amount of heat released by the ethane. To do this, we calculate the number of moles of ethane gas using the ideal gas equation and multiply the molar heat of combustion by the number of moles.

\[ \Delta H_{\text{combustion}} = 1437.17 \text{ kJ/mol} \]

\[ n = \frac{PV}{RT} \]

\[ n = \frac{0.95 \times 6.7}{0.08314 \times 298} \]

\[ n = 0.2569 \text{ mol} \]

Heat released by ethane:

\[ q = (1437.17 \text{ kJ/mol}) \times 0.2569 \text{ mol} = 369.21 \text{ kJ} \]

Then using the heat equation we can find the mass of water that would be raised to boiling with the given amount of heat. First, the kJ must be converted to J to match the units of the specific heat.

\[ 369210 = (m)(4.184)(373-298) \]

Using basic algebra we solve for the mass, and since water has a density of 1.0 g/cm^3, the mass will be equal to the volume.

\[ M = 1176.58 \text{ g} \]
Volume of water: 1.177 L

\[ w = -\Delta(PV) \]

- \( w \) = Work
- \( P \) = Pressure
- \( V \) = Volume

**Q2**

A balloon filled with gas expands under a constant pressure of \( 2.0 \text{ \times 10}^5 \) Pascals from a volume of 5.0 L to 10 L.

**Solution**

\[
\text{work} = -\text{Pressure} \times \Delta\text{Volume} \\
= -\text{pressure} \times (V_{\text{final}} - V_{\text{initial}}) = -2\times10^5 \times (10-5) \text{ Pa} \times \text{L} = -10^6 \text{ Pa} \times \text{L} = -1000 \text{ J} = -1.0 \text{ kJ of work}
\]

\[
E = q + W \\
E = \text{Energy} \\
q = \text{Heat} \\
W = \text{Work}
\]

**Q3**

A balloon filled with gas expands its volume by 2.0 L. If the pressure outside the balloon is 0.93 bar and the energy change of the gas is 450 J, how much heat did the surroundings give the balloon?

**Solution**

Remember that 100 Joule = 1 L*bar.

\[
450 = q - (0.93)(2.0)100 \]

Now solving for \( q \)

\[
q = 636 \text{ J}
\]

**Q4**

There is a house hold heater that operates at 4 V and at 35 Ω and is used to heat up 15 g of copper wire. The specific heat capacity of copper is 24.440 J/(mol K). How much time is required to increase the temperature from 25°C to 69°C?
Solution

It is important to know the equation in circuitry that calculates power: \( P = \frac{V^2}{R} \), which is derived from the equation \( V = IR \). We will also be using \( q = mc_\varphi \Delta T \).

\[
[P=\frac{V^2}{R}]
\]

\( P \) is power in units of J/s
- \( V \) is voltage in volts
- \( R \) is resistance in Ω

\[ P = \frac{(4)^2}{35} = .457 \text{ J/s} \]
\[ q = (15)(24.440)(69-25) = 16130.4 \text{ J} \]

We now know how many joules of heat must be added to the copper wire to increase the temperature and we know how many joules of energy are given off by the heater per second. We divide to find the number of seconds.

\[ \frac{(16130.4 \text{ J})}{(.457 \text{ J/s})} = 35296.3 \text{ seconds} \]

\[
\ln\left(\frac{P_1}{P_2}\right) = \frac{\Delta H_{\text{vap}}}{R} \left[\left(\frac{1}{T_2}\right) - \left(\frac{1}{T_1}\right)\right]
\]

\( P_1 \) and \( P_2 \) refer to the pressures in any unit (bar, atmosphere, Pascal)
\( R \) is the gas constant that correlates with the pressure and temperature units used.
\( T_1 \) and \( T_2 \) refer to the temperatures in Kelvin

Q5

If the temperature of a water bath closed system is raised from room temperature to 65 °C and the initial pressure is 350 torr, what is the final pressure of the system? The heat of vaporization of liquid water is 43.99 kJ/mol.

Solution

The gas constant that is most convenient to use is 8.314 J/K/mol. Therefore it is important to convert the kJ value of the heat of vaporization to J.

\[
\ln\left(\frac{350}{P_2}\right) = \frac{43990}{8.314} \left(\frac{1}{298} - \frac{1}{338}\right)
\]

Using basic algebra and the knowledge that \( e^{\ln(x)} = x \), we can solve for \( P_2 \).

\[ P_2 = 42.8 \text{ torr} \]

Q6

Given a Carnot engine that absorbs 750 J of energy from a tank of hot water with a final temperature of 300 K, what is the initial temperature if 600 J of work was done by the system?
Solution

\[ \varepsilon = \frac{T_H - T_L}{T_H} = \frac{w}{q} \]

- \( \varepsilon \) = efficiency
- \( T_H \) and \( T_L \) are the temperatures in Kelvin
- \( w \) is work in J
- \( q \) is heat in J

Set the two equivalent expressions equal to one another:

\[ \frac{T_H - 300}{T_H} = \frac{600}{750} \]

Using basic algebra solve for the initial temperature.

\[ T_H = 1500 \text{ K} \]

Q7

If 0.2 moles of hydrogen gas occupies an inflexible container with a capacity of 45 mL and the temperature is raised from 25°C to 30°C, what is the change in pressure of the contained gas, assuming ideal behavior?

Solution

\[ PV = nRT \]

- \( P \) is Pressure
- \( V \) is Volume
- \( n \) is the number of moles present in the sample
- \( R \) is the gas constant
- \( T \) is temperature in Kelvins

Using the ideal gas law and knowing four of the five variables, it is possible to solve for the fifth variable. It is important to note that while the equation is mostly correct, but it is only perfectly accurate if the gas is ideal.

In order to find a change in pressure, you must first find both your initial pressure, \( P_1 \) and your final pressure, \( P_2 \), than you must subtract \( P_1 \) from \( P_2 \). This can be simplified by solving the ideal gas law for pressure, then subtracting initial conditions from final conditions.

\[ P = \frac{nRT}{V} \]

or

\[ \Delta P = \frac{nR(T_2 - T_1)}{V} \]

Since \( R \) (0.008314 L bar/molK) is in liters and Kelvin, you must first divide 45 by 1000 to convert to mL, for a value of
0.045 L. Then convert both temperatures to Kelvin by 273.15, for values of 298.15 K and 303.15 K. Or, since the degree size is the same in Celsius and Kelvin, you can simply subtract 25 from 30 for a difference of 5 C = 5 K.

\[
\Delta P = \frac{0.2\text{mol}(0.008314\text{Lbar/molK})(5 \text{ K})}{0.045\text{L}} = 0.184756 \text{ bar}
\]

### Enthalpy

**ΔH = Σ [Products - Reactants]**

ΔH = Change in Enthalpy (for reaction)

Products = elements and compounds on the right side of the chemical equation

Reactants = elements and compounds on the left side of the chemical equation

#### Q8

Using standard thermodynamic values, calculate the change in enthalpy of reaction (ΔH\(_{\text{rxn}}\)) in the formation of liquid water from hydrogen and oxygen gas.

**Solution**

Chemical Equation:

\[
\text{H}_2(\text{g}) + \frac{1}{2}\text{O}_2(\text{g}) \rightarrow \text{H}_2\text{O}(\text{l}) + \text{heat}
\]

**Product:**

ΔH\(_f\) \text{H}_2\text{O}(\text{l}) = -285.83 \text{ kJ/mol}

**Reactants:**

ΔH\(_f\) \text{H}_2(\text{g}) = 0 \text{ kJ/mol} (the ΔH\(_f\) of elements in their standard state is defined to be 0 kJ)

ΔH\(_f\) \text{O}_2(\text{g}) = 0 \text{ kJ/mol} \times 2

Use ΔH of formation (H\(_f\)) for each of the chemicals involved in the reaction found in a standard table or reference book.

\[
\Delta H_{\text{rxn}} \text{SUM} \frac{(-285.83 \text{ kJ}) - ((\frac{1}{2})\times0 \text{ kJ} + 0 \text{ kJ})}{= -285.83 \text{ kJ/mol}}
\]

#### Q9

Using standard thermodynamic values, calculate the enthalpy of the reaction of the combustion of methane gas with oxygen gas to form carbon dioxide and liquid water.

**Solution**

Chemical Equation:
\[ CH_4(g) + 2 O_2(g) \rightarrow CO_2(g) + 2 H_2O(l) + \text{heat} \]

**Products:**
\[
\Delta H_f H_2O(l) = -285.83 \text{ kJ/mol} \times 2 \\
\Delta H_f CO_2(g) = -393.51 \text{ kJ/mol} 
\]

**Reactants:**
\[
\Delta H_f CH_4(g) = -74.87 \text{ kJ/mol} \\
\Delta H_f O_2(g) = 0 \text{ kJ/mol} \times 2 
\]

Use values found in a standard table or reference book.

\[
[2*(\Delta H_f H_2O(l) = -285.83 \text{ kJ/mol}) + \Delta H_f CO_2(g) = -393.51 \text{ kJ/mol}] \\
- [2*(\Delta H_f O_2 = 0 \text{ kJ/mol}) + (\Delta H_f CH_4 = -74.87 \text{ kJ/mol})] = \\
\Delta H_{rxn} = [2*(-285.83 \text{ kJ}) + (-393.51 \text{ kJ})] - [(2*0 \text{ kJ}) + (-74.87 \text{ kJ})] = -890.3 \text{ kJ/mol} 
\]

**Q10**

How much heat is released when burning 0.5 kg of liquid rubbing alcohol (2-propanol)? Products are carbon dioxide and liquid water. Assume an excess of oxygen.

**Solution**

**Chemical Reaction:**

\[ 2 \text{C}_3\text{H}_8\text{O}(l) + 9 \text{O}_2(g) \rightarrow 6 \text{CO}_2(g) + 8 \text{H}_2\text{O}(l) + \text{heat} \]

0.5 kg propanol * (1 mol / 60.084 g) = 8.3 mols propanol

\[
\Delta H_{rxn} = [\text{products} - \text{reactants}] = [6*(-393.51 \text{ kJ}) + 8*(-285.83 \text{ kJ})] - [(2*0 \text{ kJ}) + 9*(-74.87 \text{ kJ})] \\
= -4011.3 \text{ kJ} / (2 \text{ mols propanol}) = -2005.65 \text{ kJ/mol} \\
-2005.65 \text{ kJ/mol} \times 8.3 \text{ mols} = -16646 \text{ kJ released as heat} 
\]

**Entropy**

\[
\Delta S_{\text{Universe}} = \Delta S_{\text{Surroundings}} - \Delta S_{\text{System}} \\
\Delta S \text{ is the change in entropy} 
\]

**Q11**

If 1.6g of CH\(_4\) reacts with oxygen gas to form water and carbon dioxide what is the change in entropy for the universe?

**Solution**

**Reaction Equation:**

\[ CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \]
To solve this problem the following equations are also necessary:

\[
\Delta S_{\text{System}} = \sum \Delta S_{\text{Products}} - \sum \Delta S_{\text{Reactants}}
\]

\[
\Delta S_{\text{System}} = [(0.21374 \text{ kJ/mol}) + (2 \times 0.06995 \text{ kJ/mol})] - [(2 \times 0.20507 \text{ kJ/mol}) + (0.18626 \text{ kJ/mol})] = -0.24276 \text{ kJ/mol}
\]

\[
\Delta H_{\text{System}} = \sum \Delta H_{\text{Products}} - \sum \Delta H_{\text{Reactants}}
\]

\[
\Delta H_{\text{System}} = [( -393.509 \text{ kJ/mol}) + (2 \times -285.83 \text{ kJ/mol})] - [(2 \times 0) + (-74.87 \text{ kJ/mol})] = -890.229 \text{ kJ/mol}
\]

\[
\Delta S_{\text{Surroundings}} = \frac{\Delta H_{\text{System}}}{T}
\]

\[
\Delta S_{\text{Surroundings}} = \frac{-890.229}{298} = -2.9873 \text{ kJ/mol}
\]

\[
\Delta S_{\text{Universe}} = \Delta S_{\text{Surroundings}} - \Delta S_{\text{System}}
\]

\[
\Delta S_{\text{Universe}} = -2.9873 \text{ kJ/mol} - (-0.24276 \text{ kJ/mol}) = -2.745 \text{ kJ/mol}
\]

\[
\Delta S = k \ln(w)
\]

\(\Delta S\) is the change in entropy
\(K\) is the Boltzmann constant in J/K/particle
\(W\) is the number of microstates possible

Q12

The volume of a gas starts at 5.0 L at a temperature of 400K and a pressure of 1.12 bar. If the change in entropy was .787 J/K/mol, what was the final volume of the gas?

Solution

Remember that the number of microstates is proportional to the volume of an ideal gas. Also, the Boltzmann constant is by particle; multiplying the gas constant by the number of moles of gas is equivalent.

\[
\Delta S = R_n \ln(V_2/V_1)
\]

\(R\) is the gas constant
\(n\) is the number of moles of gas
\(V_2\) and \(V_1\) are volumes in L

\[
.787 = (8.314)n \ln(V_2/5.0)
\]

Now to find the number of moles we use the ideal gas law:

\[
n = \frac{PV}{RT}
\]

\[
n = \frac{[1.12 \times 5.0]}{[8.314 \times 400]}
\]

Now plug this value into the original equation and solve for the final volume.

\[
V_2 = 8.77 \text{ L}
\]

\[
\Delta S_{\text{Rxn}} = \sum \Delta S_{\text{Products}} - \sum \Delta S_{\text{Reactants}}
\]
Q13

Calculate the change in entropy for the dissociation of \( \text{HCl}^{(aq)} \) to \( \text{H}^+ \) and \( \text{Cl}^- \).

Solution

First, you must write out the full equation.

\[ \text{HCl}^{(aq)} \rightarrow \text{H}^+^{(aq)} + \text{Cl}^-^{(aq)} \]

Next, look up each compound in a thermodynamic table and plug the values into the equation.

\[ \Delta S_{\text{System}} = (56.6 + 0) \text{ J/molK} - 186.9 \text{ J/molK} = -130.3 \text{ J/molK} \]

Gibbs Free Energy

\[ K = e^{[-\Delta G/RT]} \]

- \( K \) is the equilibrium constant
- \( e \) is the numerical value 2.718
- \( \Delta G \) is the change in Gibbs free energy in J/mol
- \( R \) is the gas constant
- \( T \) is the temperature in K

Q14

What is the equilibrium constant for the formation of \( \text{N}_2\text{O}_4 \) gas from \( \text{NO}_2 \) gas molecules? The temperature of the reaction is 310.5K.

Solution

First, the balanced equation must be written:

\[ 2\text{NO}_2(g) \rightarrow \text{N}_2\text{O}_4(g) \]

Now using thermodynamic values for enthalpy and entropy, the Gibbs free energy can be calculated.

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

Remember that the total change in enthalpy or entropy is the sum of the change in enthalpies/entropies of the products minus the sum of the change in enthalpies/entropies of the reactants.

\[ \Delta H_{\text{System}} = \Sigma \Delta H_{\text{Products}} - \Sigma \Delta H_{\text{Reactants}} \]

\[ \Delta H_{\text{System}} = [9.08 \text{ kJ/mol}] - [2 \times 33.1 \text{ kJ/mol}] = -57.12 \text{ kJ/mol} \]

\[ \Delta S_{\text{System}} = \Sigma \Delta S_{\text{Products}} - \Sigma \Delta S_{\text{Reactants}} \]
\[ \Delta S_{\text{System}} = [0.30438 \text{ kJ/molK}] - [2 \times 0.24004 \text{ kJ/molK}] = -0.1757 \text{ kJ/molK} \]

Also, the \( T \) used is not room temperature, but the temperature given in the problem – the temperature at which the reaction takes place.

\[ \Delta G = \Delta H - T \Delta S \]
\[ \Delta G = [-57.12] - 310.5[-0.1757] = -2.565 \text{ kJ/mol or -2565 J/mol} \]

Once \( \Delta G \) is calculated the original equation can be used to solve for \( k \).

\[ K = e^{\frac{-\Delta G}{RT}} \]
\[ K = e^{\frac{-2565}{8.314 \times 310.5}} = 2.701 \]

\[ \Delta G = \Delta H - T \Delta S \]
\[ \Delta G \] is the change in Gibbs Free Energy for the reaction
\[ \Delta H \] is the change in enthalpy for the reaction
\[ \Delta S \] is the change in entropy for the reaction
\[ T \] is the temperature in Kelvin

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**Q15**

Find the change is Gibbs Free Energy for the reaction of hydrochloric acid and sodium hydroxide to form liquid water and sodium chloride at 31 C.

**Solution**

First you must write the chemical equation for the reaction: \( \text{HCl(aq) + NaOH(aq) -> H}_2\text{O(l) + NaCl} \)

Next, you must calculate \( \Delta H \) and \( \Delta S \) for the reaction.

\[ \Delta H_{\text{Rxn}} = \Sigma \Delta H_{\text{Products}} - \Sigma \Delta H_{\text{Reactants}} \]
\[ \Delta H_{\text{Rxn}} = [(285.8 + (-411.54)) \text{ kJ/mol}] - [(-167.16 + (-470.1)) \text{ kJ/mol}] = -60.05 \text{ kJ/mol} \]

\[ \Delta S_{\text{Rxn}} = \Sigma \Delta S_{\text{Products}} - \Sigma \Delta S_{\text{Reactants}} \]
\[ \Delta S_{\text{Rxn}} = [(0.06991 + 0.07238) \text{ kJ/molK}] - [0.0565 + 0.0482 \text{ kJ/molK}] = 0.03759 \text{ kJ/molK} \]

Next, the temperature must be converted to Kelvins by 273.15 to its value in Celsius.

\[ 31 + 273.15 = 304.15 \text{ K} \]

Finally, all of these values are plugged into the original equation, \( \Delta G = \Delta H - T \Delta S \).

\[ \Delta G = -60.05 \text{ KJ/mol} - 304.15 \text{ K} \times (0.03759 \text{ KJ/molK}) = -71.4830 \]

There also exist equations to correct for the temperature dependence of \( \Delta H \) and \( \Delta S \), but they are not commonly used because the difference is typically very slight. They are:
ΔH(T) = ΔH°_{rxn} - \int C_p \, dT
ΔS(T) = ΔS°_{rxn} - \int C_p \, dT

If you need to use these equations for an extremely accurate value of ΔG, simply solve these equations for ΔH and ΔS, then plug these values into the equation for ΔG.

Outside Links

- www.chemtables.tk -- A useful website table containing many thermodynamic properties of various elements and compounds

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