Combustion Chemistry 2025 **Exercise 1** **Herman Andersson**
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Task 1: For a given change in enthalpy (ΔH) and change in entropy (ΔS), determine if the reaction is going to be spontaneous or non-spontaneous and qualitatively show it on the plot area provided below. If the reaction changes from spontaneous to non-spontaneous (or vice versa) at some temperature (T), calculate the temperature value and mark it on the plot.

(a) $\Delta H = +85$ kJ/mol and $\Delta S = +300$ J/mol K

(b) $\Delta H = -150$ kJ/mol, $\Delta S = +200$ J/mol K and $T = 298$ K, calculate ΔG

(c) $\Delta H = +75$ kJ/mol and $\Delta S = -100$ J/mol K and $T = 298$ K, calculate ΔG

(d) $\Delta H = -100$ kJ/mol and $\Delta S = -250$ J/mol K

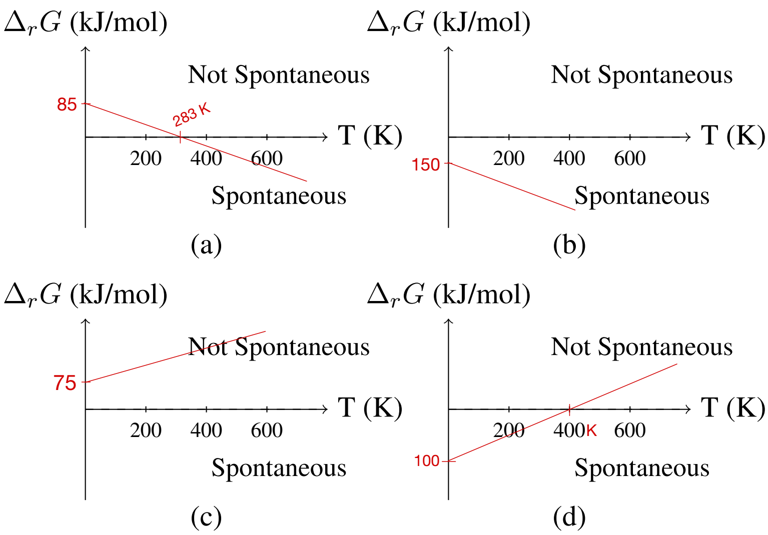
Anwser: By calculating the Gibs energy $\Delta G = \Delta H – \Delta TS$ and seeing if the values reach zero for any temperature will show if the reaction at any point goes from spontaneous to non-spontaneous. If $\Delta G > 0$, the reaction reaction will be non-spontaneous. If $\Delta G < 0$, the reaction reaction will be spontaneous. For our four cases, the calculations and figures are presented below.

(a) $\Delta H > 0$ and $\Delta T > 0$ will result in a shift for ΔG, will go from non-spontaneous to spontaneous at higher temperatures
$\Delta G = \Delta H – \Delta ST \rightarrow 0 = 85 * 10^3 - 300 * T \rightarrow T = 283.33K \approx 283K$

(b) $\Delta H < 0$ and $\Delta T > 0$ will always result in $\Delta G < 0$, will always be spontaneous
$\Delta G = \Delta H – \Delta ST \rightarrow G = -150 * 10^3 - 200 * 298K \rightarrow G = -209.6$ kj/mol

(c) $\Delta H > 0$ and $\Delta T < 0$ will always result in $\Delta G > 0$, will always be non-spontaneous
$\Delta G = \Delta H – \Delta ST \rightarrow G = +75 * 10^3 - (-100) * 298K \rightarrow G = 104.8$ kj/mol

(D) $\Delta H < 0$ and $\Delta T < 0$ will result in a shift for ΔG, will go from spontaneous to non-spontaneous at higher temperatures
$\Delta G = \Delta H – \Delta ST \rightarrow 0 = -100 * 10^3 - (-250) * T \rightarrow T \approx 400K$



Task 2: The reaction of 1 mole of Methane (CH_4) with 2 moles of air (O_2 + $3.76N_2$) results in 1 mole of carbon dioxide (CO_2), 2 moles of water (H_2O) and 7.52 moles of (N_2). Calculate the mole and mass fraction of product species. Also, determine mole and mass fraction of air in the reactant mixture.

Atomic weights: C is 12.011 amu, H is 1 amu, O is 16 amu and N is 14 amu.

Total number of moles of product = $n_{O_2} + n_H + n_{N_x}$

$\sum X_i = 1$ and $\sum Y_i = 1$ for species i = 1 to n

Anwser: We want to first calculate X_i and Y_i for all products and reactant air. We also perform a check of $\sum X_i = 1$ to ensure that the present amount of materials match up.

Product Calculations

$X_i = \frac{n_i}{n_tot}$ $n_{tot,prod} = n_{CO_2} + n_{H_2O} + n_{N2} = 1 + 2 + 7.52 = 10.52$ mol

$X_{CO_2} = \frac{1}{10,52} = 0.095 // X_{H_2O} = \frac{2}{10,52} = 0.190 // X_{N_2} = \frac{7.52}{10,52} = 0.715$

$\sum(X_i) = X_{CO_2} + X_{H_2O} + X_{N_2} = 1$

Calculation of the total mass:

$m_{tot} = W_{CO_2} * n_{CO_2} + W_{H_2O} * n_{H_2O} + W_{N_2} * n_{N_2} = 44.011 * 1 + 18 * 2 + 28 * 7.52 = 290.571g$

Calculation of mass fractions:

$Y = \frac{m_i}{m_{tot}} \rightarrow Y_{CO_2} = \frac{m_{CO_2}}{m_{tot}} = \frac{44.011}{290.571} = 0.151 // Y_{H_2O} = \frac{m_{H_2O}}{m_{tot}} = \frac{36}{290.571} = 0.124 // Y_{N_2} = \frac{m_{N_2}}{m_{tot}} = \frac{210.56}{290.571} = 0.725$

Air Calculations

$\sum(n_i) = n_{tot,rec} = n_{CH_4} + X_{air} = 1 + 2 = 3$ mol

$X_{CH_4} = \frac{1}{3} = 0.33 // X_{air} = \frac{2}{3} = 0.66$

Molecular weight is equal to the sum of all present atoms in the molecule. For methane the molecular weight is $W_{CH_4} = 12.011 * 1 + 4 * 1 = 16.011 \frac{g}{mol}$ and for air it's $W_{air} = \frac{1}{\frac{0.21}{32} + \frac{0.79}{28}} = 28.86 \frac{g}{mol}$

Calculation of the molecular weight of mixtrue:

$m_{tot} = W_{CH_4} * x_{CH_4} + W_{air} * x_{air} = 44.011 * 0.33 + 28.86 * 0.66 = 33.57 \frac{g}{mol}$

Mass fraction of air in reactant mixture: $Y_{air} = \frac{X_{air} * W_{air}}{W_{mix}} = \frac{0.66 * 28.86}{33.57} = 0.567$

Task 3: The piston of a vertical piston-cylinder device containing a gas has a mass of 60 kg and a cross-sectional area of 0.04 m^2. The local atmospheric pressure is 0.97 bar. Furthermore, the piston is subjected to gravitational acceleration is 9.81 m/s^2.

Hint: The Piston is frictionless.

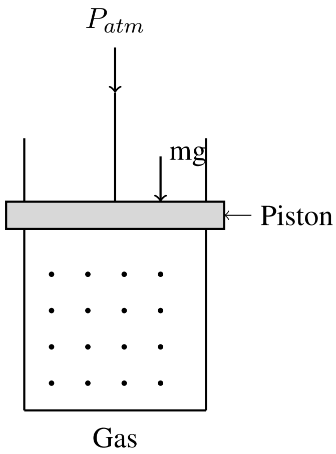


Figure 1: Vertical piston-cylinder device

(a) Determine the pressure inside the cylinder

To calculate the pressure inside the cylinder, we can use the fact that the pressure inside the cylinder must match the pressure excreted above the piston. The force balance equation from this situationen becomes the following

Pressure inside column = Pressure on column $\rightarrow p_{cylinder} * A = p_{atm} * A * m * g$

$p_{cylinder} = p_{atm} + \frac{m*g}{A} = 0.97 * 10^5 + \frac{60*9.81}{0.04} = 111715[pa] = 1.12[bar]$

(b) If some heat is transferred to the gas, what will happen to the pressure and volume inside the cylinder?

When heat is introduced into the system, the gas will try to expand. Cause the piston is frictionless, it will move with the expansion, leading to an increase volume inside the cylinder. As long as the piston don't exert more force against the gas, the pressure will remain the same.

In summary, volumne will increase and pressure will increase as the same.