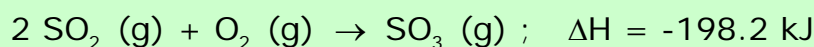


THERMOCHEMISTRY: EXERCISES

1. The main process in the production of the sulfuric acid (contact method) is the catalytic oxidation of sulfur dioxide at a temperature of 400 °C



- How much heat is released in the oxidation of 74.6 g of sulfur dioxide at constant pressure?
- Predict the change in entropy
- Explain why an decrease in temperature will favor the spontaneity of the process

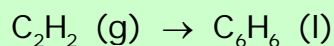
Molar mass: sulfur dioxide = 64 g /mol

2. Let's suppose that gasoline is pure octane, $\text{C}_8 \text{H}_{18}$.

- Write the balanced equation of the combustion of gasoline
- Determine the heat released (in kJ) when 40 kg of gasoline are burned.
- Determine the mass of CO_2 , in kilograms, produced in that combustion

Atomic weights: C=12; O=16. Formation enthalpies:
 $\text{H}_2\text{O} (\text{g}) = -242 \text{ kJ/mol}$; $\text{CO}_2 (\text{g}) = -394 \text{ kJ/mol}$; $\text{C}_8\text{H}_{18} (\text{l}) = -250 \text{ kJ/mol}$

3. Benzene liquid, C_6H_6 , can be obtained at $p=15 \text{ atm}$ and $T=25 \text{ °C}$ from acetylene, C_2H_2 , as expressed in this non-balanced equation:

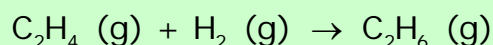


The enthalpy change of the process is -631 kJ/mol . Determine:

- The molar enthalpy of the combustion reaction of $\text{C}_6\text{H}_6 (\text{l})$ from the molar enthalpy of combustion of acetylene, which is -1302.1 kJ/mol
- The volume of acetylene, at 25 °C and 0.5 atm , needed to obtain 0.25 L of benzene

$R = 0.082 \text{ atm}\cdot\text{L}/\text{K}\cdot\text{mol}$. Density of benzene = 0.95 kg/L
Atomic weights: C=12, O=16, H=1

4. Ethane can be produced by hydrogenation of ethene:



From the following values

	C₂H₄ (g)	H₂ (g)	C₂H₆ (g)
ΔH_f° (kJ/mol)	52.3	-	-84.9
S° (J/K.mol)	209	130.6	229

determine the enthalpy and entropy changes for the reaction and determine if the reaction is spontaneous at 25 °C

5. The combustion of acetylene, C₂H₂ (g) produces carbon dioxide and water

a) Describe the chemical equation

b) Determine then molar enthalpy change of the combustion of acetylene and the heat released when 1 kg of acetylene is burned

Standard formation enthalpies: acetylene=+223.75 kJ/mol;
carbon dioxide (g) = -393.5 kJ/mol; water (g) = -241.8 kJ/mol

SOLUTIONS TO THE PROBLEMS

① (a) $Q_p = \Delta H = -\frac{198.2 \text{ kJ}}{2 \text{ mol SO}_2} \times \frac{1 \text{ mol SO}_2}{64 \text{ g SO}_2} \times 74.6 \text{ g SO}_2$

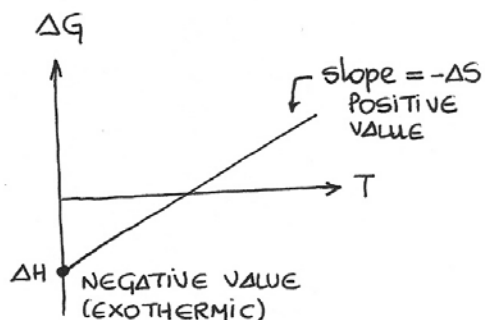
$Q_p = \Delta H = -115.5 \text{ kJ}$... heat released at constant pressure

- (b) All reactants and products are gases but the atoms (matter) are more "ordered" packed in the molecules of products. Therefore,

$$S_{\text{prod}} < S_{\text{react}}$$

$\Delta S = S_{\text{prod}} - S_{\text{react}} < 0$... prediction: the change in entropy is negative

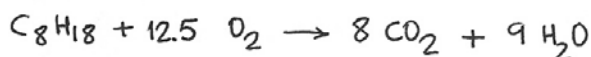
- (c) According to the prediction made



Decrease in T favors spontaneity because ΔG is more negative in that direction

$$T \downarrow \quad \Delta G \downarrow$$

- ② (a) The balanced equation



(b) $\Delta H_{\text{comb}}(\text{octane}) = 8 \times \Delta H_f^\circ(\text{CO}_2) + 9 \times \Delta H_f^\circ(\text{H}_2\text{O}) - \Delta H_f^\circ(\text{C}_8\text{H}_{18})$

$$\Delta H_{\text{comb}}(\text{octane}) = -3152 \text{ kJ} - 2178 \text{ kJ} + 250 \text{ kJ}$$

$$\Delta H_{\text{comb}}(\text{octane}) = -5080 \text{ kJ/mol C}_8\text{H}_{18}$$

$$M(\text{octane}) = (8 \times 12) + (18 \times 1) = 114 \text{ g/mol}$$

$$\Delta H = 40000 \text{ g} \times \frac{1 \text{ mol}}{114 \text{ g}} \times \frac{(-5080 \text{ kJ})}{1 \text{ mol}} = -1.78 \times 10^6 \text{ kJ}$$

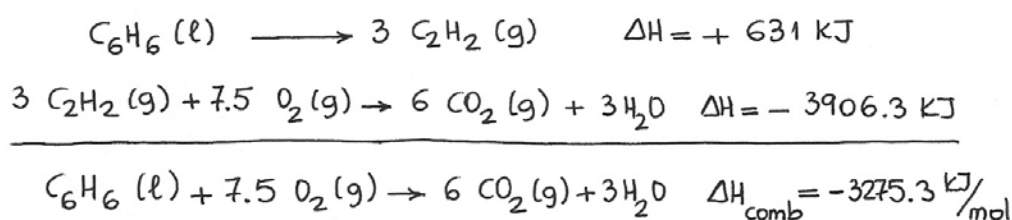
- (c)

$$m(\text{CO}_2) = 40000 \text{ g C}_8\text{H}_{18} \times \frac{1 \text{ mol C}_8\text{H}_{18}}{114 \text{ g C}_8\text{H}_{18}} \times \frac{8 \text{ mol CO}_2}{1 \text{ mol C}_8\text{H}_{18}} \times \frac{44 \text{ g CO}_2}{1 \text{ mol CO}_2} \times \frac{1 \text{ kg}}{1000 \text{ g}} =$$

$$= 123.5 \text{ kg CO}_2$$

$$M(\text{CO}_2) = 12 + (2 \times 16) = 44 \text{ g/mol}$$

③ a) Applying Hess's Law



b) From this balanced equation



$$m(\text{C}_6\text{H}_6) = 0.25 \text{ L} \times \frac{950 \text{ g}}{1 \text{ L}} = 237.5 \text{ g benzene}$$

$$n(\text{C}_2\text{H}_2) = 237.5 \text{ g C}_6\text{H}_6 \times \frac{3 \text{ mol C}_2\text{H}_2}{78 \text{ g C}_6\text{H}_6} = 9.13 \text{ mol C}_2\text{H}_2 \text{ are needed}$$

$$M(\text{C}_6\text{H}_6) = (6 \times 12) + (6 \times 1) = 78 \text{ g/mol}$$

Applying the general equation of gases:

$$\begin{aligned}
 PV = nRT \rightarrow V &= \frac{nRT}{P} = \frac{9.13 \text{ mol} \times 0.082 \text{ atmL/kmol} \times 298 \text{ K}}{0.5 \text{ atm}} = \\
 &= 446.2 \text{ L C}_2\text{H}_2(\text{g}) \text{ are needed}
 \end{aligned}$$

④ Enthalpy change

$$\Delta H_{\text{rxn}}^{\circ} = \Delta H_f^{\circ}(\text{C}_2\text{H}_6) - \Delta H_f^{\circ}(\text{C}_2\text{H}_4) - \Delta H_f^{\circ}(\text{H}_2) = -137.2 \text{ kJ (exothermic)}$$

Entropy change

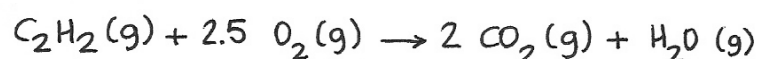
$$\Delta S^{\circ} = S^{\circ}(\text{C}_2\text{H}_6) - S^{\circ}(\text{C}_2\text{H}_4) - S^{\circ}(\text{H}_2) = -110.6 \text{ J/K (the system becomes more ordered)}$$

Spontaneity at 25°C

$$\Delta G = \Delta H - T \times \Delta S = -137200 \text{ J} + 110.6 \frac{\text{J}}{\text{K}} \times 298 \text{ K} = -104241 \text{ J}$$

$\Delta G < 0 \rightarrow$ the reaction is spontaneous at 25°C

⑤ a) The chemical equation (balanced):



b) The molar enthalpy change of combustion of acetylene

$$\Delta H_c(\text{C}_2\text{H}_2) = 2 \times \Delta H_f^\circ(\text{CO}_2) + \Delta H_f^\circ(\text{H}_2\text{O}) - \Delta H_f^\circ(\text{C}_2\text{H}_2)$$

$$\Delta H_c(\text{C}_2\text{H}_2) = -787 \text{ kJ} - 241.8 \text{ kJ} - 223.75 \text{ kJ} = -1252.55 \text{ kJ}$$

$$\Delta H_c(\text{C}_2\text{H}_2) = -1252.55 \text{ kJ/mol}$$

Heat when 1 Kg of C_2H_2 is burned

$$M(\text{C}_2\text{H}_2) = (2 \times 12) + (2 \times 1) = 26 \text{ g/mol}$$

$$Q_p = \Delta H = 1000 \text{ g C}_2\text{H}_2 \times \frac{-1252.55 \text{ kJ}}{1 \text{ mol C}_2\text{H}_2} \times \frac{1 \text{ mol C}_2\text{H}_2}{26 \text{ g C}_2\text{H}_2}$$

$$Q_p = \Delta H = -48175 \text{ kJ}$$