

## **Topic 6.**

### **CHEMICAL THERMODYNAMICS**

#### **Theoretical QUESTIONS for preparation:**

##### **1. The First Law of Thermodynamics**

- A. A system, surroundings, work, heat
- B. The first law of thermodynamics
- C. Internal energy
- D. Endothermic and exothermic processes

##### **2. Enthalpy**

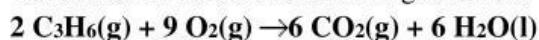
- A. Reaction enthalpy
- B. Hess' law and standard enthalpy of formation

##### **3. The second law of thermodynamics and entropy**

##### **4. Free-energy changes**

### **TASKS**

1. Calculate  $\Delta H_{rxn}^0$  for the following reaction:



If  $\Delta H^0(\text{C}_3\text{H}_6(\text{g})) = 20.9 \text{ kJ/mol}$ ,  $\Delta H^0(\text{CO}_2(\text{g})) = -393.2 \text{ kJ/mol}$ ,  $\Delta H^0(\text{H}_2\text{O}(\text{l})) = -286 \text{ kJ/mol}$ .

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**ANSWER:** \_\_\_\_\_

2. Calculate  $\Delta H^0$  for  $2\text{Al(s)} + \text{Cr}_2\text{O}_3\text{(s)} \rightarrow \text{Al}_2\text{O}_3\text{(s)} + 2\text{Cr(s)}$ .  
If  $\Delta H^0(\text{Cr}_2\text{O}_3\text{(s)}) = -1128 \text{ kJ/mol}$ ;  $\Delta H^0(\text{Al}_2\text{O}_3\text{(s)}) = -1676 \text{ kJ/mol}$ .

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**ANSWER:** \_\_\_\_\_

3. Given the following entropy values (Al<sub>2</sub>O<sub>3</sub>(s) is 51.00 J/K\*mol; Al(s) is 28.32 J/K\*mol; H<sub>2</sub>O(g) is 188.7 J/K\*mol; H<sub>2</sub>(g) is 130.6 J/K\*mol), determine  $\Delta S$  for the reaction:

$$\text{Al}_2\text{O}_3(\text{s}) + 3\text{H}_2(\text{g}) \rightarrow 2\text{Al}(\text{s}) + 3\text{H}_2\text{O}(\text{g})$$

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**ANSWER:** \_\_\_\_\_

4. Reaction at 25C: **6C(graphite) + 3H<sub>2</sub>(g) → C<sub>6</sub>H<sub>6</sub>(l)**.

Entropy contents (S) (J/mol\*K):

C(graphite) = 5.74

H<sub>2</sub>(gas) = 130.68

C<sub>6</sub>H<sub>6</sub>(l) = 172.8

Calculate entropy change.

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**ANSWER:** \_\_\_\_\_

5. Calculate  $\Delta G^\circ$  for the reactions of complete glucose oxidation ( $C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$ ) under standard conditions if  $\Delta G^\circ$  for each reaction are given:

$$\Delta G^\circ(C_6H_{12}O_6) = -910 \text{ kJ/mol}$$

$$\Delta G^\circ(O_2) = 0 \text{ kJ/mol}$$

$$\Delta G^\circ(CO_2) = -394 \text{ kJ/mol}$$

$$\Delta G^\circ(H_2O) = -237 \text{ kJ/mol}$$

Will the process run spontaneously?

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**ANSWER:** \_\_\_\_\_

6. Reaction has a  $\Delta H = +5600$  calories. The entropy change is  $-4.6$  calories /Kelvin at 298 Kelvin. Is this reaction spontaneous?

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**ANSWER:** \_\_\_\_\_

7. Calculate the free energy change for the complete combustion of one mole of methane,  $\text{CH}_4(\text{g})$ , the main component of natural gas:  $\text{CH}_4(\text{g}) + 2 \text{ O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g}) + 2 \text{ H}_2\text{O}(\text{l})$ . Use the table below. Is this reaction spontaneous?

Substance	$^{\circ}\text{H}$ , kJ/mol	$^{\circ}\text{S}$ , J/K*mol
CH <sub>4</sub> (g)	-74.86	186.19
O <sub>2</sub> (g)	0	205.03
CO <sub>2</sub> (g)	-393.5	213.7
H <sub>2</sub> O (l)	-285.84	69.96

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