

## 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

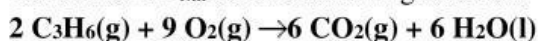
- A. Reaction enthalpy
- B. Hess' law and standard enthalpy of formation

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

##### 4. Free-energy changes

#### TASKS

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



If  $\Delta H^0(\text{C}_3\text{H}_{6(\text{g})}) = 20.9 \text{ kJ/mol}$ ,  $\Delta H^0(\text{CO}_{2(\text{g})}) = -393.2 \text{ kJ/mol}$ ,  $\Delta H^0(\text{H}_2\text{O}_{(\text{l})}) = -286 \text{ kJ/mol}$ .

#### GIVEN:

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#### QUESTION: \_\_\_\_\_

#### FORMULA:

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**CALCULATIONS:**

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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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**QUESTION:** \_\_\_\_\_

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**CALCULATIONS:**

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

3. Given the following entropy values ( $\text{Al}_2\text{O}_3(\text{s})$  is  $51.00 \text{ J/K}\cdot\text{mol}$ ;  $\text{Al}(\text{s})$  is  $28.32 \text{ J/K}\cdot\text{mol}$ ;  $\text{H}_2\text{O}(\text{g})$  is  $188.7 \text{ J/K}\cdot\text{mol}$ ;  $\text{H}_2(\text{g})$  is  $130.6 \text{ J/K}\cdot\text{mol}$ ), 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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**QUESTION:** \_\_\_\_\_

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**CALCULATIONS:**

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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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**QUESTION:** \_\_\_\_\_

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**CALCULATIONS:**

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

5. Calculate  $\Delta G^\circ$  for the reactions of complete glucose oxidation ( $\text{C}_6\text{H}_{12}\text{O}_6 + 6\text{O}_2 \rightarrow 6\text{CO}_2 + 6\text{H}_2\text{O}$ ) under standard conditions if  $\Delta G^\circ$  for each reaction are given:

$\Delta G^\circ(\text{C}_6\text{H}_{12}\text{O}_6) = -910 \text{ kJ/mol}$

$\Delta G^\circ(\text{O}_2) = 0 \text{ kJ/mol}$

$\Delta G^\circ(\text{CO}_2) = -394 \text{ kJ/mol}$

$\Delta G^\circ(\text{H}_2\text{O}) = -237 \text{ kJ/mol}$

Will the process run spontaneously?

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**QUESTION:** \_\_\_\_\_

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**CALCULATIONS:**

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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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**QUESTION:** \_\_\_\_\_

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**CALCULATIONS:**

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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	$\Delta H$ , kJ/mol	$\Delta S$ , J/K $\cdot$ 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

**GIVEN:**

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**QUESTION:** \_\_\_\_\_

**FORMULA:**

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**CALCULATIONS:**

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