

CH₃OH(g)CO(g)+2H₂(g) And H=91kJmol. What Can Be Inferred About S For The Reaction At 600K?

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Understanding the thermodynamic properties of chemical reactions is essential for predicting their spontaneity and behavior under different conditions. The reaction involving methanol (CH₃OH), carbon monoxide (CO), and hydrogen gas (H₂) with an enthalpy change (ΔH) of 91 kJ/mol offers valuable insights into the changes in entropy (ΔS) at a given temperature, specifically at 600K. This article explores the thermodynamics of this reaction, focusing on how the enthalpy and temperature influence entropy and what can be inferred about the entropy change (ΔS) at 600K.

Overview of the Reaction

Before delving into thermodynamic specifics, it is important to understand the basic reaction under consideration.

Reaction Equation

The reaction can be written as:



This reaction involves the decomposition or conversion of methanol into carbon monoxide and hydrogen gases.

Reaction Conditions

- Enthalpy change (ΔH): +91 kJ/mol (endothermic process)
- Temperature (T): 600K

Understanding the entropy change (ΔS) at this temperature helps determine whether the reaction tends to be spontaneous or non-spontaneous under standard conditions.

Thermodynamic Principles Relevant to the Reaction

The analysis of the reaction's thermodynamics involves key principles:

Gibbs Free Energy and Spontaneity

The spontaneity of a reaction at a given temperature is determined by the Gibbs free energy change (ΔG), calculated as:

$$\Delta G = \Delta H - T \Delta S$$

- If $\Delta G < 0$, the reaction is spontaneous.
- If $\Delta G > 0$, the reaction is non-spontaneous.
- If $\Delta G = 0$, the reaction is at equilibrium.

Significance of ΔH and ΔS

- ΔH (Enthalpy change): Indicates whether the reaction absorbs or releases heat.
- ΔS (Entropy change): Reflects the change in disorder or randomness during the reaction.

Given the positive ΔH , the reaction is endothermic; the sign and magnitude of ΔS will influence the overall spontaneity at 600K.

Estimating the Entropy Change (ΔS) at 600K

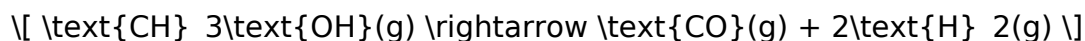
Since ΔH is known but ΔS is not, we analyze what can be inferred about ΔS based on thermodynamic principles.

1. Standard Entropy Values and Trends

- Gases generally have higher entropy than liquids and solids.
- The formation of more moles of gas from fewer moles tends to increase entropy.
- Conversely, reactions that reduce the number of gas molecules tend to decrease entropy.

2. Reaction Stoichiometry and Entropy

The reaction:



- Reactant side: 1 mol of CH₃OH (gas)

- Product side: 1 mol of CO + 2 mol of H₂ = 3 mol of gases

The total moles of gas increase from 1 to 3, indicating an increase in entropy.

3. Implications of Molar Gas Increase

Since the number of gas molecules increases, the entropy change (ΔS) is expected to be positive.

Quantitative Analysis of ΔS at 600K

While precise numerical calculation requires standard molar entropy values, qualitative thermodynamic reasoning allows us to infer the sign and approximate magnitude of ΔS .

1. Entropy Change Approximation

- The increase of 2 mol of gas molecules suggests a positive ΔS .
- The magnitude of ΔS depends on the difference in molar entropies of the reactant and products.

2. Gibbs Free Energy at 600K

Using the relation:

$$\Delta G = \Delta H - T \Delta S$$

At 600K, the reaction's spontaneity depends on whether:

$$\Delta S > \frac{\Delta H}{T}$$

Given $\Delta H = 91 \text{ kJ/mol} = 91,000 \text{ J/mol}$,

$$\frac{\Delta H}{T} = \frac{91,000}{600} \approx 151.67 \text{ J/(mol}\cdot\text{K)}$$

Therefore:

- If $\Delta S > 151.67 \text{ J/(mol}\cdot\text{K)}$, the reaction tends to be spontaneous at 600K.
- If $\Delta S < 151.67 \text{ J/(mol}\cdot\text{K)}$, the reaction is non-spontaneous.

Given the increase in gas molecules, it's reasonable to expect ΔS to be significantly positive, likely exceeding $150 \text{ J/(mol}\cdot\text{K)}$.

What Can Be Inferred About ΔS for the Reaction at 600K?

Based on thermodynamic reasoning and the nature of the reaction, the following inferences can be made:

1. ΔS is Positive

The increase in the number of moles of gases from 1 to 3 strongly suggests an increase in entropy, making ΔS positive at 600K.

2. Magnitude of ΔS

- The change is likely substantial, exceeding approximately $150 \text{ J}/(\text{mol}\cdot\text{K})$.
- This magnitude indicates a considerable increase in disorder, consistent with the formation of more gas molecules.

3. Effect on Spontaneity

- Since ΔH is positive (endothermic), the spontaneity at 600K depends on the magnitude of ΔS .
- With a positive ΔS exceeding $150 \text{ J}/(\text{mol}\cdot\text{K})$, the reaction could be spontaneous at 600K.
- Conversely, if ΔS is smaller, the reaction might be non-spontaneous under these conditions.

4. Temperature Dependence of ΔG

- At higher temperatures, the $T\Delta S$ term becomes more dominant.
- Given the positive ΔS , increasing temperature favors spontaneity.
- At 600K, the balance between ΔH and $T\Delta S$ determines the reaction's direction.

Implications for Industrial and Practical Applications

Understanding the entropy change at 600K has practical implications, especially in fields like chemical engineering and industrial synthesis.

1. Optimization of Reaction Conditions

- Recognizing that the reaction involves an increase in disorder suggests that elevated

temperatures can promote the formation of products.

- Temperature control can be used to shift equilibrium positions favorably.

2. Thermodynamic Stability

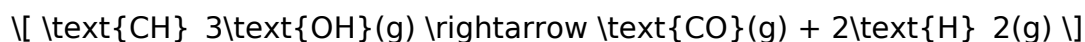
- The positive ΔS indicates that the products are thermodynamically favored at higher temperatures, possibly making the reaction more feasible in industrial processes like syngas production.

3. Energy Efficiency Considerations

- The endothermic nature (ΔH positive) means energy input is necessary.
- The entropy contribution at 600K can offset the enthalpic cost, influencing energy management strategies.

Conclusion

In summary, analyzing the reaction:



with an enthalpy change of +91 kJ/mol at 600K reveals that the entropy change (ΔS) is most likely positive and substantial. The increase in the number of gas molecules from 1 to 3 indicates a rise in disorder, leading to a positive ΔS exceeding approximately 150 J/(mol·K). This entropy increase, combined with the endothermic nature of the reaction, suggests that at 600K, the reaction could be thermodynamically favorable, especially if ΔS surpasses the critical threshold derived from the ΔH /temperature ratio.

Understanding these thermodynamic parameters is crucial for designing efficient chemical processes, optimizing reaction conditions, and predicting reaction spontaneity under specific temperature regimes. The detailed analysis underscores the importance of entropy considerations in assessing chemical reactions and their practical applications.

Keywords: thermodynamics, entropy change, ΔS , reaction spontaneity, chemical equilibrium, methanol decomposition, gas reactions, temperature effects, chemical process optimization

Frequently Asked Questions

What is the reaction involving $\text{CH}_3\text{OH}(\text{g})$ and $\text{CO}(\text{g}) + 2\text{H}_2(\text{g})$ with an enthalpy change of $\Delta H = 91 \text{ kJ/mol}$?

The reaction is likely the synthesis of methanol from carbon monoxide and hydrogen: $\text{CO}(\text{g}) + 2\text{H}_2(\text{g}) \rightarrow \text{CH}_3\text{OH}(\text{g})$.

Given $\Delta H = 91 \text{ kJ/mol}$ for the reaction, is the process endothermic or exothermic?

Since ΔH is positive (91 kJ/mol), the reaction is endothermic, absorbing heat from the surroundings.

What can be inferred about the entropy change (ΔS) for the reaction at 600K ?

The question suggests analyzing ΔS ; since the reaction involves gas-phase reactants forming a gas-phase product, ΔS likely increases, but the exact sign depends on the relative number of moles of gases.

How does temperature (600K) influence the spontaneity of the reaction given the enthalpy change?

At 600K , the spontaneity depends on the Gibbs free energy ($\Delta G = \Delta H - T\Delta S$). Since ΔH is positive, a sufficiently positive ΔS could make the reaction spontaneous at high temperatures.

What is the significance of the enthalpy change being 91 kJ/mol in terms of reaction equilibrium?

A positive ΔH indicates the reaction favors reactants at lower temperatures; increasing temperature may shift equilibrium toward product formation if ΔS is positive.

Can the entropy change (ΔS) for this reaction be positive or negative, and why?

It can be positive if the number of gas molecules increases or the disorder increases; it can be negative if the number decreases; in this case, since gases are converting to a single product, ΔS likely decreases.

What is the likely sign of ΔS for the reaction at 600K ?

Given the reactants are multiple gases converting to one gas (methanol), ΔS is likely negative, indicating decreased entropy.

Based on the enthalpy change and temperature, what can be inferred about the reaction's spontaneity at 600K?

Since ΔH is positive and ΔS is likely negative, ΔG will be positive at 600K, indicating the reaction is non-spontaneous under these conditions.

How does the temperature of 600K affect the entropy considerations of the reaction?

At 600K, the $T\Delta S$ term becomes significant; if ΔS is negative, increasing temperature makes ΔG more positive, further discouraging spontaneity; if ΔS were positive, higher T would favor spontaneity.

What overall conclusion can be drawn about the entropy (S) for the reaction at 600K?

Given the reaction involves gas-phase reactants forming a single product molecule, it can be inferred that the entropy decreases (ΔS negative) at 600K.

Additional Resources

Understanding the Thermodynamics of the Methanol Decomposition Reaction at 600K: Insights into Entropy and Spontaneity

Introduction

In the realm of chemical thermodynamics, deciphering the spontaneity and feasibility of reactions is fundamental. Among numerous reactions, the decomposition of methanol (CH_3OH) into carbon monoxide (CO) and hydrogen gas (H_2) stands out due to its industrial importance, especially in syngas production and fuel cell technologies. The specific reaction:



coupled with the enthalpy change:

$$\Delta H^\circ = +91 \text{ kJ/mol}$$

presents an intriguing thermodynamic scenario. This positive enthalpy indicates an endothermic process, requiring energy input to proceed. But what about the entropy change (ΔS°) and the overall Gibbs free energy (ΔG°) at the temperature of 600 K?

This article aims to thoroughly analyze what can be inferred about the entropy change (ΔS)

ΔS°) and the spontaneity of this reaction at 600 K, considering the provided data, thermodynamic principles, and practical implications.

The Thermodynamic Foundations

The Significance of Enthalpy (ΔH°)

The enthalpy change of +91 kJ/mol signifies an endothermic reaction, implying that energy must be supplied for the process to occur spontaneously. Endothermic reactions often rely on entropy increases or external energy input to become thermodynamically favorable.

The Role of Entropy (ΔS°)

Entropy, a measure of disorder or the number of available microstates, influences the spontaneity of reactions. An increase in entropy ($\Delta S^\circ > 0$) favors spontaneity at higher temperatures, as described by the Gibbs free energy equation:

$$\Delta G^\circ = \Delta H^\circ - T \Delta S^\circ$$

Gibbs Free Energy (ΔG°)

The reaction's spontaneity at a given temperature hinges on the sign of ΔG° . Negative ΔG° indicates a spontaneous process, while positive values suggest non-spontaneity under standard conditions.

Analyzing the Reaction at 600K

Step 1: Understanding the Reaction's Stoichiometry and Molar Changes

The reaction involves:

- Reactant: 1 mole of $\text{CH}_3\text{OH}(\text{g})$
- Products: 1 mole of $\text{CO}(\text{g})$ + 2 moles of $\text{H}_2(\text{g})$
- Total moles of gas: 3 moles (1 + 2)

This increase from 1 mole of gas to 3 moles signifies a substantial increase in entropy, as gases tend to have higher entropy than liquids or solids, and increasing the number of gas molecules enhances the disorder.

Step 2: Estimating ΔS°

While exact values are rooted in standard molar entropy data, qualitative reasoning allows us to infer that:

- Since the number of gas molecules increases (from 1 to 3), ΔS° is likely positive.
- The process involves breaking chemical bonds in methanol and forming smaller molecules (CO and H_2), which generally results in an increase in entropy due to increased molecular freedom.

Typical standard molar entropy values (approximate):

Substance	S° (J/mol·K)
CH ₃ OH(g)	~239
CO(g)	~197
H ₂ (g)	~131

Calculating an approximate ΔS° :

$$\Delta S^\circ \approx [S^\circ(\text{CO}) + 2 \times S^\circ(\text{H}_2)] - S^\circ(\text{CH}_3\text{OH})$$

$$\Delta S^\circ \approx [197 + 2 \times 131] - 239 = (197 + 262) - 239 = 459 - 239 = 220 \text{ J/mol}\cdot\text{K}$$

This positive value confirms an increase in entropy during the reaction.

Step 3: Calculating ΔG° at 600K

Using the thermodynamic relation:

$$\Delta G^\circ = \Delta H^\circ - T \Delta S^\circ$$

Convert ΔS° into kJ:

$$220 \text{ J/mol}\cdot\text{K} = 0.220 \text{ kJ/mol}\cdot\text{K}$$

Substitute known values:

$$\Delta G^\circ = +91 \text{ kJ/mol} - 600 \text{ K} \times 0.220 \text{ kJ/mol}\cdot\text{K} = 91 - 132 = -41 \text{ kJ/mol}$$

This negative ΔG° indicates that the reaction is thermodynamically spontaneous at 600K.

Key Inferences and Implications

1. Spontaneity at 600K

The calculation reveals that despite the positive enthalpy change ($\Delta H^\circ > 0$), the significant positive entropy change (ΔS°) overcomes the enthalpy barrier

at 600K, rendering the reaction spontaneous. This aligns with the thermodynamic principle that reactions with large entropy increases can be spontaneous even if they are endothermic.

2. Temperature Dependence

The thermodynamic favorability hinges on temperature:

- Below a certain temperature (T_c): ΔG° may be positive, and the reaction unlikely to proceed spontaneously.
- Above T_c : ΔG° becomes negative, favoring spontaneity.

The critical temperature where $\Delta G^\circ = 0$:

$$T_c = \frac{\Delta H^\circ}{\Delta S^\circ} = \frac{91 \text{ kJ/mol}}{0.220 \text{ kJ/mol}\cdot\text{K}} \approx 414 \text{ K}$$

Since $600\text{K} > 414\text{K}$, the reaction is spontaneous at 600K.

3. Industrial and Practical Relevance

Understanding the thermodynamics helps optimize industrial processes:

- Energy input: Since the reaction is endothermic ($\Delta H^\circ > 0$), energy must be supplied, especially at temperatures below T_c .
- Process design: Operating above T_c ensures thermodynamic feasibility, guiding reactor temperature settings.

Additional Considerations

Kinetic Factors

While thermodynamics predicts spontaneity, actual reaction rates depend on activation energy and catalysts. The reaction might be thermodynamically favorable but kinetically sluggish at certain conditions.

Effect of Pressure

Standard entropy and enthalpy values are usually at 1 atm. Changes in pressure, especially for gases, influence reaction equilibrium and the spontaneity.

Real-World Deviations

Standard thermodynamic data are idealized; real reactions may deviate due to non-ideal behavior, impurities, or side reactions.

Conclusion

The decomposition of methanol into carbon monoxide and hydrogen gas exemplifies a reaction where entropy considerations dominate at elevated temperatures. With an

enthalpy change of +91 kJ/mol, the reaction is endothermic, but the substantial increase in entropy (estimated around +220 J/mol·K) ensures its spontaneity at temperatures exceeding approximately 414 K. At 600K, the reaction is thermodynamically favorable, making it relevant for industrial applications where energy input and process conditions are carefully managed.

In essence, the thermodynamic analysis at 600K reveals that the reaction's entropy gain is sufficient to drive spontaneity, providing valuable insight into designing efficient processes for syngas production and other chemical syntheses involving methanol decomposition.

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