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Understanding the spontaneity of a chemical reaction is fundamental in thermodynamics. When provided with the enthalpy change (ΔH_rxn), the entropy change (ΔS_rxn), and the temperature (T), chemists can determine whether a reaction will occur spontaneously under specific conditions. In this article, we will explore how to calculate the change in the universe's entropy (ΔSuniv), which indicates the overall tendency of a process to proceed spontaneously, using the given values: ΔH_rxn = 84 KJ, ΔS_rxn = 144 J/K, and T = 300 K.

Fundamentals of Thermodynamics in Chemical Reactions

Understanding Key Concepts

Before delving into calculations, it’s important to understand the core thermodynamic principles involved:

- **Enthalpy Change (ΔH_rxn):** Represents the heat absorbed or released during a reaction at constant pressure. A positive ΔH_rxn indicates an endothermic process, while a negative value indicates exothermicity.
- **Entropy Change (ΔS_rxn):** Measures the change in disorder or randomness in a system during the reaction. An increase in entropy favors spontaneity.
- **Temperature (T):** The temperature at which the reaction occurs, measured in Kelvin (K).

Significance of ΔSuniv (Change in Universe Entropy)

The second law of thermodynamics states that for a process to be spontaneous, the total entropy of the universe must increase:

$$
\Delta S_{univ} = \Delta S_{system} + \Delta S_{surroundings} > 0
$$

Calculating ΔSuniv helps determine whether the reaction will proceed spontaneously under the given conditions.

Calculating ΔSuniv

Step 1: Convert All Values to Consistent Units

Given:
- $\Delta H_{rxn} = 84$ KJ
- $\Delta S_{rxn} = 144$ J/K
- $T = 300$ K

Since ΔH_{rxn} is provided in kilojoules, convert it to joules:

$$
\Delta H_{rxn} = 84\, \text{KJ} \times 1000\, \text{J/KJ} = 84,000\, \text{J}
$$

Now, both ΔH_{rxn} and ΔS_{rxn} are in joules, ensuring consistency in calculations.

Step 2: Calculate the Entropy Change of the Surroundings ($\Delta S_{surroundings}$)

The entropy change of the surroundings is related to the heat exchange with the system:

$$
\Delta S_{surroundings} = -\frac{\Delta H_{rxn}}{T}
$$

The negative sign indicates that when the system absorbs heat (endothermic), the surroundings lose entropy, and vice versa.

Substituting the values:

$$
\Delta S_{surroundings} = -\frac{84,000\, \text{J}}{300\, \text{K}} = -280\, \text{J/K}
$$

Step 3: Calculate the Total Change in Universe Entropy (ΔSuniv)

Now, sum the entropy changes:

$$
\Delta S_{univ} = \Delta S_{rxn} + \Delta S_{surroundings}
$$

\]

\[
\Delta S_{univ} = 144\, \text{J/K} + (-280\, \text{J/K}) = -136\, \text{J/K}
\]

Interpretation: Since ΔSuniv is negative, the reaction under these conditions is non-spontaneous. The universe's total entropy decreases, which violates the second law of thermodynamics.

Evaluating Thermodynamic Spontaneity

Understanding the Implications of the Calculation

The negative value of ΔSuniv suggests that, at 300 K, this reaction does not proceed spontaneously. This aligns with thermodynamic principles: for a reaction to be spontaneous, ΔSuniv must be greater than zero.

Step 4: Analyzing the Effect of Temperature

If the reaction is endothermic (positive ΔH_rxn) and has a positive ΔS_rxn, increasing temperature can make ΔSuniv positive.

The general criterion for spontaneity:

\[
\Delta G_{rxn} = \Delta H_{rxn} - T \Delta S_{rxn} < 0
\]

And the relation to universe entropy:

\[
\Delta S_{univ} = -\frac{\Delta G_{rxn}}{T}
\]

Therefore, to find the temperature at which the reaction becomes spontaneous (ΔSuniv > 0):

\[
\Delta G_{rxn} < 0 \Rightarrow \Delta H_{rxn} - T \Delta S_{rxn} < 0
\]

Rearranged:

\[
T > \frac{\Delta H_{rxn}}{\Delta S_{rxn}}
\]

Plugging in the values:

$$
T > \frac{84,000\, \text{J}}{144\, \text{J/K}} \approx 583.33\, \text{K}
$$

Conclusion: The reaction becomes spontaneous at temperatures above approximately 583.33 K, indicating that higher temperatures favor spontaneity for this endothermic, entropy-increasing process.

Real-World Applications of Thermodynamic Calculations

Predicting Reaction Feasibility in Industrial Processes

Engineers and chemists use calculations like these to determine whether a chemical process is thermodynamically favorable under specific conditions. For example, designing energy-efficient manufacturing processes requires understanding how temperature influences spontaneity.

Designing Thermally Controlled Reactions

By adjusting temperature, industries can optimize reaction yields, minimize energy consumption, and improve safety. Knowing the critical temperature thresholds ensures reactions are conducted under conditions that maximize efficiency.

Environmental Impact Assessments

Calculating ΔSuniv helps assess whether reactions can occur naturally or require energy input, aiding in evaluating environmental impacts or designing sustainable processes.

Summary and Key Takeaways

- Convert all thermodynamic values to consistent units before calculations.
- The entropy change of the surroundings can be derived from the enthalpy change and temperature.
- For the reaction at 300 K, the overall universe entropy decreases, indicating non-spontaneity under these conditions.
- Spontaneity can be achieved at higher temperatures, specifically above

approximately 583 K for this reaction.

- Understanding these principles helps in process design, optimizing reaction conditions, and predicting reaction behavior.

Final Thoughts

Determining the spontaneity of a chemical reaction through thermodynamic calculations provides valuable insights into its feasibility. By analyzing ΔH_rxn, ΔS_rxn, and T, chemists can predict whether a process will proceed naturally or require intervention. In the case discussed, the reaction is not spontaneous at 300 K, but increasing the temperature beyond 583 K can make it favorable. Mastery of these calculations is essential for scientists and engineers working to develop efficient, sustainable, and safe chemical processes.

Frequently Asked Questions

How do you calculate the change in Gibbs free energy (ΔG) using Hrxn, Srxn, and temperature T?

Use the Gibbs free energy equation: ΔG = Hrxn - T × Srxn. Ensure units are consistent; convert Srxn from J/K to KJ/K if necessary.

Given Hrxn = 84 KJ, Srxn = 144 J/K, and T = 300 K, what is the ΔG for the reaction?

Convert Srxn to KJ/K: 144 J/K = 0.144 KJ/K. Then, ΔG = 84 KJ - 300 K × 0.144 KJ/K = 84 KJ - 43.2 KJ = 40.8 KJ.

What does a positive ΔG indicate about the spontaneity of the reaction at 300 K?

A positive ΔG (40.8 KJ) indicates that the reaction is non-spontaneous at 300 K under standard conditions.

How do you calculate the entropy of the universe (Suniv) using ΔH, ΔS, and ΔG?

Since Suniv = ΔS_universe = ΔS_system + ΔS_surroundings, and ΔG = ΔH - TΔS, for a process at equilibrium, Suniv can be assessed by checking the sign of ΔG and related entropy changes.

Is the reaction spontaneous or non-spontaneous at 300 K based on the given data?

Since ΔG is positive (40.8 KJ), the reaction is non-spontaneous at 300 K.

How does temperature influence the spontaneity of a reaction given specific ΔH and ΔS values?

Temperature influences spontaneity because ΔG = ΔH - TΔS. If ΔH and ΔS are positive, increasing T may make ΔG negative, favoring spontaneity; if negative, the opposite occurs.

Can you determine whether the universe's entropy increases or decreases for this reaction at 300 K?

Since the reaction is non-spontaneous (positive ΔG), the total entropy of the universe decreases or remains unchanged; more detailed calculations of ΔS_universe would be needed for precise determination.

What are the key steps to analyze spontaneity and universe entropy change with given thermodynamic data?

First, calculate ΔG using ΔH, ΔS, and T. Next, determine if ΔG is negative (spontaneous). Then, analyze entropy changes in surroundings to assess Suniv. A negative ΔG generally correlates with an increase in universe entropy.

Additional Resources

Given the Values of ΔHrxn, ΔSrxn, and T Below, Determine ΔSuniv

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Introduction

Thermodynamics forms the backbone of understanding chemical reactions and their spontaneity. The concept of entropy, enthalpy, and temperature converge to determine whether a process will naturally proceed in a given direction. A fundamental thermodynamic quantity, the change in the universe's entropy (ΔSuniv), indicates the spontaneity of a process: if ΔSuniv > 0, the process is spontaneous; if ΔSuniv < 0, it is non-spontaneous; and if ΔSuniv = 0, the system is at equilibrium.

In this article, we focus on a specific problem: Given the values of enthalpy change (ΔHrxn), entropy change (ΔSrxn), and temperature (T), how do we calculate the entropy change of the universe (ΔSuniv)?

Specifically, we examine the scenario where:

- ΔHrxn = 84 kJ
- ΔSrxn = 144 J/K
- T = 300 K

This detailed analysis aims to illustrate the principles and calculations involved, providing a comprehensive understanding suitable for students, educators, and researchers interested in thermodynamics.

Fundamental Concepts in Thermodynamics

Before delving into calculations, it is crucial to review the core thermodynamic principles involved:

1. Enthalpy Change (ΔHrxn)

- Represents the heat absorbed or released during a reaction at constant pressure.
- Positive ΔHrxn (endothermic) indicates heat absorption.
- Negative ΔHrxn (exothermic) indicates heat release.

2. Entropy Change (ΔSrxn)

- Measures the disorder or randomness of the system.
- A positive ΔSrxn suggests increased disorder.
- A negative ΔSrxn indicates decreased disorder.

3. The Universe's Entropy Change (ΔSuniv)

- Defined as:

$$
ΔSuniv = ΔS_{system} + ΔS_{surroundings}
$$

- The second law of thermodynamics states:

$$
ΔSuniv \geq 0
$$

with equality at equilibrium.

Calculating ΔSuniv: The Core Approach

Given the problem data, the key challenge lies in evaluating ΔSuniv based on the known ΔHrxn, ΔSrxn, and T.

The general relation is:

$$
\Delta Suniv = \Delta S_{universe} = \Delta S_{system} + \Delta S_{surroundings}
$$

Since the system's entropy change is known (ΔSrxn), the remaining component is the entropy change of the surroundings (ΔSsurroundings), which depends on the heat exchange with the system.

1. Relationship Between Enthalpy and Surroundings

The surroundings are often considered as a large thermal reservoir at temperature T, which exchanges heat with the system. The entropy change of the surroundings is:

$$
\Delta S_{surroundings} = -\frac{Q_{system}}{T}
$$

where:

- Q_{system} is the heat absorbed or released by the system.

- The negative sign accounts for the fact that heat gained by the system is lost by the surroundings, and vice versa.

For reactions at constant pressure:

$$
Q_{system} = \Delta H_{rxn}
$$

Therefore:

$$
\Delta S_{surroundings} = -\frac{\Delta H_{rxn}}{T}
$$

This relation assumes the surroundings are large enough to maintain constant temperature T during the process.

Step-by-Step Calculation

Using the above relation, the calculation proceeds as follows:

$$
\Delta Suniv = \Delta S_{rxn} + \Delta S_{surroundings}
$$

$$
\Delta Suniv = \Delta S_{rxn} - \frac{\Delta H_{rxn}}{T}
$$

\]

Converting Units for Consistency

Ensure all quantities are in compatible units:

- ΔHrxn = 84 kJ = 84,000 J
- ΔSrxn = 144 J/K
- T = 300 K

Calculation of ΔSuniv

Plugging the values into the formula:

\[
ΔSuniv = 144\, \text{J/K} - \frac{84,000\, \text{J}}{300\, \text{K}}
\]

\[
ΔSuniv = 144\, \text{J/K} - 280\, \text{J/K}
\]

\[
ΔSuniv = -136\, \text{J/K}
\]

Result: The entropy change of the universe is −136 J/K.

Interpretation of the Result

The negative value of ΔSuniv indicates that, under the given conditions, the process is non-spontaneous. This conclusion aligns with the thermodynamic criterion:

- When ΔSuniv < 0, the process tends to proceed in the reverse direction or is thermodynamically unfavorable at the specified temperature.

Deeper Thermodynamic Insights

While the calculation straightforwardly shows a negative ΔSuniv, a comprehensive analysis involves examining the individual contributions and their implications.

1. Spontaneity and Gibbs Free Energy

The relationship between ΔHrxn, ΔSrxn, and spontaneity is often expressed via the Gibbs free energy change (ΔG):

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

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

Given the data:

$$
\Delta G = 84{,}000\, \text{J} - 300\, \text{K} \times 144\, \text{J/K} = 84{,}000\, \text{J} - 43{,}200\, \text{J} = 40{,}800\, \text{J}
$$

Since $\Delta G > 0$, the process is non-spontaneous at 300 K, consistent with the negative ΔSuniv.

2. Temperature Dependence

The sign of ΔG and ΔSuniv can change with temperature:

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

- Equilibrium at the temperature where $\Delta G = 0$:

$$
T_{eq} = \frac{\Delta H}{\Delta S} = \frac{84{,}000\, \text{J}}{144\, \text{J/K}} \approx 583.33\, \text{K}
$$

- For $T < 583.33$ K, $\Delta G > 0 \Rightarrow$ non-spontaneous.
- For $T > 583.33$ K, $\Delta G < 0 \Rightarrow$ spontaneous.

Given $T = 300$ K < 583.33 K, the process remains non-spontaneous at this temperature, aligning with the negative ΔSuniv.

Broader Implications and Context

The analysis exemplifies how thermodynamic parameters dictate reaction spontaneity and the importance of considering both enthalpy and entropy contributions. It also emphasizes the critical role of temperature in shifting the balance between spontaneity and non-spontaneity.

Practical Considerations in Thermodynamics

In real-world scenarios, the environment’s heat exchange, reaction conditions, and phase considerations can influence the actual process. While the theoretical calculations provide clear thermodynamic insights, experimental factors may modify the observed outcomes.

Summary of Key Points

- The entropy change of the universe (ΔSuniv) is computed as:

$$
ΔSuniv = ΔS_{rxn} - \frac{ΔH_{rxn}}{T}
$$

- Using the provided data, ΔSuniv = −136 J/K, indicating a non-spontaneous process at 300 K.
- The process's spontaneity depends on temperature; it is spontaneous only when T > 583.33 K.
- Gibbs free energy analysis confirms the non-spontaneity at 300 K, since ΔG > 0.

Conclusion

Determining the entropy change of the universe based on reaction enthalpy, entropy change, and temperature provides essential insights into the thermodynamic favorability of processes. The calculation demonstrates the interplay between heat exchange and disorder, emphasizing the importance of temperature in thermodynamic spontaneity.

The scenario analyzed exemplifies fundamental principles that underpin modern thermodynamics, offering a framework for evaluating reactions in both academic and practical contexts. Whether in chemical manufacturing, environmental science, or materials engineering, understanding these concepts enables scientists and engineers to predict and control reaction outcomes effectively.

References

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- Zumdahl, S. S., & DeCoste, D. J. (2010). Chemical Principles. Cengage Learning.
- Levine, I. N. (2014). Quantum Chemistry. Pearson Education.

Note: All calculations are based on standard thermodynamic relations, assuming ideal behavior and constant pressure conditions.

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