

The Value Of S For The Catalytic Hydrogenation Of Acetylene To Ethene, $\text{C}_2\text{H}_2(\text{g}) + \text{H}_2(\text{g}) \rightarrow \text{C}_2\text{H}_4(\text{g})$ is _____

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Understanding the thermodynamic properties involved in chemical reactions is crucial for chemists and chemical engineers. Among these properties, entropy (denoted as S) plays a significant role in determining the spontaneity and feasibility of reactions. Specifically, in catalytic hydrogenation processes—such as converting acetylene (C_2H_2) to ethene (C_2H_4)—the change in entropy provides valuable insight into the reaction's thermodynamic favorability. This article explores the concept of entropy change (ΔS) for the hydrogenation of acetylene to ethene, delving into the fundamental principles, detailed calculations, and practical implications relevant to industrial and laboratory settings.

Understanding Entropy (S) in Chemical Reactions

What Is Entropy?

Entropy (S) is a thermodynamic quantity that measures the degree of disorder or randomness within a system. In chemical reactions, entropy reflects the dispersion of energy and matter, indicating how the arrangement of molecules changes during the reaction process.

Key points about entropy:

- Higher entropy corresponds to greater disorder.
- Entropy tends to increase in spontaneous processes.
- It is a state function, meaning it depends only on the initial and final states, not on the path taken.

Why Is Entropy Important?

Entropy influences the Gibbs free energy change (ΔG), which determines whether a reaction proceeds spontaneously:

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

where:

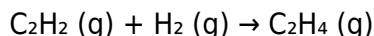
- ΔH is the enthalpy change,
- T is the temperature in Kelvin,
- ΔS is the entropy change.

A negative ΔG indicates a spontaneous reaction. Therefore, understanding the entropy change helps predict reaction direction and efficiency, especially in catalytic processes like hydrogenation.

Hydrogenation of Acetylene to Ethene: The Reaction Overview

Reaction Equation

The catalytic hydrogenation of acetylene to ethene can be summarized as:



This reaction involves adding hydrogen across the triple bond in acetylene, resulting in ethene. It is widely used in the petrochemical industry to control acetylene impurities and produce ethene for polymerization.

Significance of the Reaction

- It is an essential step in refining processes.
- The reaction is typically carried out over a metal catalyst such as palladium or nickel.
- Understanding thermodynamic parameters like ΔS guides the optimization of reaction conditions for maximum yield and efficiency.

Calculating the Entropy Change (ΔS) for the Reaction

Principles of Calculation

The entropy change for the reaction can be calculated using standard molar entropy values (S°) of reactants and products:

$$\Delta S^\circ_{\text{reaction}} = \sum S^\circ_{\text{products}} - \sum S^\circ_{\text{reactants}}$$

This involves:

- Obtaining standard molar entropy values for each species involved,
- Applying stoichiometric coefficients,
- Calculating the difference.

Standard Molar Entropy Values

Standard molar entropies (S°) are tabulated at 1 bar (or 1 atm) and a specified temperature, often 25°C (298.15 K). Typical values (approximate) are:

Species	S° (J/mol·K)
C ₂ H ₂ (g)	200.9
H ₂ (g)	130.6
C ₂ H ₄ (g)	219.0

Note: Actual values may vary slightly depending on data sources, but these are representative.

Calculating ΔS for the Reaction

Using the above data:

$$\Delta S^\circ = [S^\circ(\text{C}_2\text{H}_4)] - [S^\circ(\text{C}_2\text{H}_2) + S^\circ(\text{H}_2)]$$

Plugging in values:

$$\Delta S^\circ = 219.0 - (200.9 + 130.6) = 219.0 - 331.5 = -112.5 \text{ J/mol}\cdot\text{K}$$

This negative value indicates a decrease in entropy during the reaction.

Interpreting the Entropy Change

Implications of a Negative ΔS

A negative ΔS suggests that the system becomes more ordered or less dispersed after the reaction. In the case of acetylene hydrogenation:

- The total number of gas molecules decreases (from 2 mol on the reactant side to 1 mol on the product side),
- The reduction in gas molecules leads to decreased entropy, aligning with the negative ΔS calculated.

Correlation with Reaction Spontaneity

While entropy decreases, the overall spontaneity depends on the Gibbs free energy change:

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

- If ΔH (enthalpy change) is sufficiently negative (exothermic), the reaction can still be spontaneous despite the decrease in entropy.
- At lower temperatures, the $T\Delta S$ term is smaller, favoring spontaneity if ΔH is negative.
- At higher temperatures, the entropy term becomes more significant, potentially making ΔG positive and the reaction non-spontaneous.

Practical Applications and Industrial Relevance

Optimizing Reaction Conditions

Understanding the entropy change helps engineers design optimal conditions:

- Temperature control is critical; lower temperatures favor the exothermic hydrogenation when ΔS is negative.

- Catalyst choice influences reaction rates and selectivity, indirectly affecting thermodynamic considerations.

Safety and Efficiency

- Recognizing the thermodynamic favorability ensures reactions proceed smoothly.
- Managing entropy considerations helps prevent undesired side reactions or incomplete conversions.

Environmental Considerations

- Efficient catalytic hydrogenation reduces waste and energy consumption.
- Thermodynamic insights contribute to greener chemical processes.

Summary and Conclusion

The entropy change (ΔS) for the catalytic hydrogenation of acetylene to ethene is approximately $-112.5 \text{ J/mol}\cdot\text{K}$, reflecting a decrease in disorder as the reaction proceeds from multiple gaseous reactants to a single gaseous product. This negative entropy change indicates a more ordered state post-reaction, primarily due to the reduction in the number of gas molecules.

Despite the decrease in entropy, the overall spontaneity of the reaction depends on the enthalpy change and temperature. The process is typically exothermic, which, combined with the entropy considerations, makes it thermodynamically favorable under appropriate conditions.

Understanding the value of ΔS is essential for optimizing industrial processes, improving catalyst design, and ensuring efficient, safe, and environmentally friendly hydrogenation reactions. Accurate thermodynamic data, including entropy values, form the backbone of process engineering and chemical manufacturing strategies.

References

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- Smith, J. M., Van Ness, H. C., & Abbott, M. M. (2005). Introduction to Chemical Engineering Thermodynamics. McGraw-Hill Education.

Note: For real-world calculations, always consult the latest thermodynamic data tables and consider temperature dependence of entropy values.

Frequently Asked Questions

What is the significance of the standard electrode potential (E°) in the catalytic hydrogenation of acetylene to ethene?

The standard electrode potential (E°) indicates the tendency of the involved species to gain or lose electrons; a more positive E° value signifies a greater tendency for reduction, which helps determine the feasibility and the catalytic efficiency of the hydrogenation process.

How does the value of S (standard potential) influence the catalytic hydrogenation of acetylene to ethene?

The value of S (standard potential) helps predict whether the hydrogenation reaction is thermodynamically favorable; a higher (more positive) S value suggests a more spontaneous conversion of acetylene to ethene under standard conditions.

Why is understanding the value of S important in industrial catalytic hydrogenation processes?

Knowing the value of S allows engineers to optimize reaction conditions, select appropriate catalysts, and improve efficiency by ensuring the reaction proceeds spontaneously and with minimal energy input.

What is the typical value of the standard potential (S) for the hydrogenation of acetylene to ethene, and what does it imply?

The standard potential for the hydrogenation of acetylene to ethene is generally positive, indicating that the reaction is thermodynamically favorable and can be efficiently catalyzed to produce ethene from acetylene.

Can the value of S be used to compare the hydrogenation of different alkynes? If so, how?

Yes, the value of S can be used to compare the thermodynamic tendencies of hydrogenation reactions for different alkynes; a more positive S value indicates a more favorable and spontaneous hydrogenation process for that particular alkyne.

Additional Resources

The Value Of S For The Catalytic Hydrogenation Of Acetylene To Ethene, $\text{C}_2\text{H}_2 (\text{g}) + \text{H}_2 (\text{g}) \rightarrow \text{C}_2\text{H}_4 (\text{g})$, Is a Critical Factor in Understanding the Thermodynamics and Efficiency of the Reaction

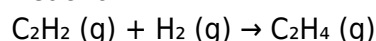
In the realm of chemical engineering and industrial chemistry, understanding the thermodynamic parameters that govern reactions is essential for optimizing processes, ensuring safety, and achieving

economic efficiency. One such parameter that often comes into focus is the standard entropy change, represented as ΔS° or simply S in some contexts. Specifically, for the catalytic hydrogenation of acetylene to ethene, the value of S —or the entropy change associated with the reaction—is a key to comprehending not just the thermodynamic feasibility but also the reaction's behavior under various conditions. This blog will explore the value of S for the catalytic hydrogenation of acetylene to ethene, its significance, how it's calculated, and the broader implications for industrial applications.

Understanding the Basics: The Reaction and Its Context

Before diving into the specifics of entropy, it's essential to understand the reaction itself:

Reaction:



- Type: Catalytic hydrogenation
- Catalyst: Typically, metals like palladium, platinum, or nickel are used
- Purpose: To convert acetylene, a common impurity in ethylene streams, into ethene, a vital feedstock in polymer production

This process is widely used in the petrochemical industry to purify ethylene streams and produce high-purity ethene for downstream polymerization processes.

The Significance of the Entropy Change (ΔS°) in Chemical Reactions

Entropy, a thermodynamic property, quantifies the degree of disorder or randomness in a system. In chemical reactions, the change in entropy (ΔS°) tells us:

- Whether the disorder increases or decreases during the reaction
- How the reaction's spontaneity is affected when combined with enthalpy (ΔH°)
- The temperature dependence of the reaction's equilibrium position

In the context of the hydrogenation of acetylene to ethene, understanding ΔS° helps chemists and engineers predict whether the reaction will proceed spontaneously under given conditions, and how the reaction equilibrium shifts with temperature.

Thermodynamic Foundations: Calculating the Standard Entropy Change

Standard Molar Entropies (S°)

Each substance involved in the reaction has a standard molar entropy value, S° , typically expressed in $\text{J}/(\text{mol}\cdot\text{K})$. These values are derived from experimental data and tabulated in thermodynamic databases.

Calculating ΔS°

The standard entropy change for the reaction is calculated as:

$$\Delta S^\circ = \sum S^\circ(\text{products}) - \sum S^\circ(\text{reactants})$$

For the hydrogenation of acetylene:

$$\Delta S^\circ = S^\circ(\text{C}_2\text{H}_4) - [S^\circ(\text{C}_2\text{H}_2) + S^\circ(\text{H}_2)]$$

Where:

- $S^\circ(\text{C}_2\text{H}_4)$ is the standard molar entropy of ethene
- $S^\circ(\text{C}_2\text{H}_2)$ is that of acetylene
- $S^\circ(\text{H}_2)$ is that of hydrogen gas

Example Data (approximate values at 25°C):

Substance	S° (J/(mol·K))
C ₂ H ₂ (g)	200
H ₂ (g)	131
C ₂ H ₄ (g)	219

Calculation:

$$\Delta S^\circ = 219 - (200 + 131) = 219 - 331 = -112 \text{ J/(mol·K)}$$

This negative ΔS° indicates a decrease in entropy during the reaction, meaning the system becomes more ordered as acetylene and hydrogen combine to form ethene.

Interpreting the Value of S: What Does It Tell Us?

Sign and Magnitude

- Negative ΔS° : The reaction results in a decrease in disorder. This is common in reactions where gaseous reactants form a more stable or more ordered product.
- Magnitude: A larger negative value suggests a significant decrease in entropy, which can influence the temperature at which the reaction is spontaneous.

Implications for Reaction Spontaneity

Using the Gibbs free energy equation:

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

- When ΔS° is negative, at higher temperatures, the $T\Delta S^\circ$ term becomes more negative, potentially making ΔG° more positive, thus less spontaneous.
- Conversely, at lower temperatures, the reaction may be spontaneous because the enthalpy term dominates.

Therefore, knowing the value of S allows engineers to determine optimal operating temperatures and

pressures to favor the formation of ethene.

Broader Industrial Significance

Process Optimization

- By understanding the entropy change, process engineers can design conditions (temperature, pressure) that maximize yield.
- In hydrogenation processes, controlling reaction thermodynamics ensures minimal side reactions and maximizes efficiency.

Safety and Control

- Reactions with large negative entropy changes often involve significant heat effects.
- Accurate thermodynamic data, including S , helps in designing safe reactors and control systems.

Environmental and Economic Impact

- Efficient hydrogenation reduces waste and energy consumption.
- Reliable thermodynamic data minimizes the risk of process failure, which can be costly and environmentally damaging.

Practical Aspects: How the Value of S Is Used

Equilibrium Calculations

Knowing ΔS° is essential for calculating the equilibrium constant (K) at different temperatures, which in turn guides the choice of operating conditions.

Reaction Kinetics and Catalysis

While thermodynamics tells us whether a reaction can occur, kinetics determine how fast. Entropy changes can influence activation energies indirectly through thermodynamic driving forces.

Catalyst Design

Understanding entropy influences catalyst selection and reactor design, ensuring that the process remains thermodynamically favorable throughout operational ranges.

Summary: The Value of S for the Hydrogenation Reaction

In conclusion, the value of S for the catalytic hydrogenation of acetylene to ethene is approximately $-112 \text{ J}/(\text{mol}\cdot\text{K})$ based on standard entropy data. This negative entropy change signifies a decrease in disorder as the gaseous reactants combine into a more ordered ethene molecule. Recognizing this helps chemists and engineers optimize conditions, predict reaction behavior, and design efficient,

safe, and environmentally friendly processes.

The precise quantification of S provides a foundation for calculating Gibbs free energy changes, equilibrium constants, and ultimately guides process parameters for industrial hydrogenation. It exemplifies how fundamental thermodynamic data underpin practical chemical engineering solutions, ensuring the production of high-purity ethene essential for polymer manufacturing and other applications.

Final Thoughts

Understanding the value of S in the hydrogenation of acetylene to ethene is more than a mere academic exercise; it is a vital component of real-world process design and optimization. As industries continue to seek greener, more efficient, and cost-effective chemical processes, mastery over thermodynamic parameters like entropy remains crucial. Whether you're a student, researcher, or industry professional, appreciating the significance of entropy changes will deepen your insight into the intricate dance of molecules that drives modern chemistry and manufacturing.

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