

For A Reaction, $\Delta H = 176 \text{ KJ/mol}$ And $\Delta S = 0.285 \text{ KJ/(Kmol)}$. At What temperatures Is This Reaction Spontaneous?

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Understanding the spontaneity of a chemical reaction is fundamental in thermodynamics and chemical kinetics. The question posed involves analyzing the conditions under which a reaction becomes thermodynamically favorable or spontaneous based on its enthalpy change (ΔH) and entropy change (ΔS). Given the values $\Delta H = 176 \text{ KJ/mol}$ and $\Delta S = 0.285 \text{ KJ/(K}\cdot\text{mol)}$, we aim to determine the temperature range at which this reaction proceeds spontaneously. This analysis involves fundamental thermodynamic principles, specifically the Gibbs free energy equation, and requires careful calculation and interpretation.

Fundamentals of Thermodynamic Spontaneity

Gibbs Free Energy and Spontaneity

The spontaneity of a chemical reaction is primarily determined by the Gibbs free energy change (ΔG). The relationship is given by:

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

Where:

- ΔG is the change in Gibbs free energy,
- ΔH is the enthalpy change,
- T is the absolute temperature in Kelvin,
- ΔS is the entropy change.

A reaction is spontaneous when $\Delta G < 0$, non-spontaneous when $\Delta G > 0$, and at equilibrium when $\Delta G = 0$.

Significance of ΔH and ΔS

- If $\Delta H < 0$ (exothermic reaction) and $\Delta S > 0$ (entropy increases), the reaction is spontaneous at all temperatures.
- If $\Delta H > 0$ (endothermic) and $\Delta S < 0$ (entropy decreases), the reaction is non-spontaneous at all temperatures.
- When both ΔH and ΔS are positive or negative, the temperature determines the spontaneity.

In our case, ΔH is positive (+176 KJ/mol), and ΔS is positive (+0.285 KJ/(K·mol)), indicating an endothermic process with increasing entropy.

Calculating the Temperature for Spontaneity

Determining the Threshold Temperature

The critical temperature ($T_{\text{spontaneous}}$) at which the reaction transitions from non-spontaneous to spontaneous is when $\Delta G = 0$:

- $0 = \Delta H - T_{\text{spontaneous}} \Delta S$

Rearranged, this becomes:

- $T_{\text{spontaneous}} = \Delta H / \Delta S$

Given:

- $\Delta H = 176 \text{ KJ/mol}$

- $\Delta S = 0.285 \text{ KJ/(K}\cdot\text{mol)}$

Note: Ensure units are consistent. Both are in KJ, so calculations are straightforward.

Calculating $T_{\text{spontaneous}}$

Plugging in the values:

$$T_{\text{spontaneous}} = 176 \text{ KJ/mol} \div 0.285 \text{ KJ/(K}\cdot\text{mol)}$$

Calculating:

$$T_{\text{spontaneous}} = (176) / (0.285) = 617.54 \text{ K}$$

Therefore, the reaction becomes spontaneous at temperatures above approximately 617.5 K.

Interpreting the Results and Spontaneity Range

Temperature Range for Spontaneity

Since both ΔH and ΔS are positive:

- The reaction is non-spontaneous at temperatures below $T_{\text{spontaneous}}$
- The reaction becomes spontaneous at temperatures above $T_{\text{spontaneous}}$

Expressed explicitly:

- Spontaneous when $T > 617.5 \text{ K}$
- Non-spontaneous when $T < 617.5 \text{ K}$

This temperature dependence aligns with thermodynamic principles, where positive ΔH and ΔS lead to a crossover point at $T_{\text{spontaneous}}$.

Implications for Practical Applications

Understanding this temperature dependence is vital for:

- Designing industrial processes that rely on such reactions
- Controlling reaction conditions to favor spontaneity
- Anticipating reaction behavior under different temperature regimes

For example, if the reaction is used in a process at 700 K, it will proceed spontaneously; at room temperature (~298 K), it will not.

Additional Considerations and Real-World Factors

Effects of Pressure and Concentration

While the thermodynamic analysis focuses on ΔH , ΔS , and T , real-world reactions also depend on:

- Pressure changes, especially for gaseous systems where entropy is pressure-dependent
- Concentration of reactants and products, influencing the reaction quotient (Q) and actual spontaneity

Limitations of the Standard Thermodynamic Approach

- The calculations assume standard conditions and ideal behavior.
- Kinetics may prevent a reaction from occurring spontaneously even if thermodynamically favorable.
- Activation energy barriers could require catalysts or external energy input.

Further Thermodynamic Analysis

- To explore how the reaction behaves at specific temperatures, one could plot ΔG against T .
- The reaction's equilibrium constant (K) can be calculated using:

$$K = e^{-\Delta G / RT}$$

where R is the gas constant and T is the temperature in Kelvin.

Summary of Key Points

1. The critical temperature at which the reaction becomes spontaneous is approximately 617.5 K.
2. Below this temperature, the reaction is non-spontaneous; above it, spontaneous.
3. This analysis relies on the Gibbs free energy equation, considering ΔH and ΔS .
4. Real-world applications must consider additional factors like pressure, concentration, and kinetics.
5. Understanding the temperature dependence aids in process optimization and control.

Conclusion

The thermodynamic analysis of the reaction with $\Delta H = 176 \text{ KJ/mol}$ and $\Delta S = 0.285 \text{ KJ/(K}\cdot\text{mol)}$ reveals a clear temperature threshold for spontaneity. Specifically, the reaction becomes thermodynamically favorable at temperatures exceeding approximately 617.5 K. This insight is essential for chemists and engineers aiming to harness or control such reactions in industrial processes, laboratory experiments, or environmental systems. By understanding the delicate balance of enthalpy and entropy

contributions, practitioners can predict and manipulate reaction pathways to achieve desired outcomes efficiently and effectively.

End of Article

Frequently Asked Questions

How do you determine the temperature at which a reaction becomes spontaneous given ΔH° and ΔS° ?

The reaction becomes spontaneous when ΔG° is negative, which occurs when $T > \Delta H^\circ / \Delta S^\circ$. So, by calculating $T = \Delta H^\circ / \Delta S^\circ$, you can find the temperature threshold.

Given $\Delta H^\circ = 176 \text{ kJ/mol}$ and $\Delta S^\circ = 0.285 \text{ kJ/(K}\cdot\text{mol)}$, what is the critical temperature for spontaneity of the reaction?

Convert units to ensure consistency: $T = \Delta H^\circ / \Delta S^\circ = 176 \text{ kJ/mol} / 0.285 \text{ kJ/(K}\cdot\text{mol)} \approx 617.54 \text{ K}$. The reaction is spontaneous at temperatures above approximately 618 K.

Why is the temperature important in determining the spontaneity of a reaction?

Because spontaneity depends on the sign of ΔG° , which is influenced by both enthalpy (ΔH°) and entropy (ΔS°) through the relation $\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ$. Temperature determines which term dominates.

If the reaction's ΔH° is positive and ΔS° is also positive, at what

temperature range is the reaction spontaneous?

The reaction is spontaneous when $T > \Delta H^\circ / \Delta S^\circ$. With positive ΔH° and ΔS° , increasing temperature favors spontaneity.

What does the sign of ΔH° and ΔS° tell us about the reaction's spontaneity at low and high temperatures?

A positive ΔH° and ΔS° suggest the reaction is non-spontaneous at low temperatures but becomes spontaneous at high temperatures when T exceeds $\Delta H^\circ / \Delta S^\circ$.

Can the reaction be spontaneous at all temperatures? Why or why not?

No, because with positive ΔH° and ΔS° , the reaction is only spontaneous above a certain temperature threshold. At temperatures below that, it is non-spontaneous.

How does the calculation of the critical temperature help in practical chemical engineering applications?

Knowing the temperature at which a reaction becomes spontaneous helps in designing reactors, controlling process conditions, and optimizing energy efficiency for industrial processes.

Additional Resources

For A Reaction, $\Delta H = 176 \text{ KJ/mol}$ And $\Delta S = 0.285 \text{ KJ/(Kmol)}$. At What Temperatures Is This Reaction Spontaneous?

Understanding the conditions under which a chemical reaction becomes spontaneous is fundamental in thermodynamics and chemical kinetics. The spontaneity of a reaction is governed primarily by its Gibbs free energy change (ΔG), which depends on both enthalpy (ΔH) and entropy (ΔS) changes. Given the thermodynamic parameters for a specific reaction—namely, an enthalpy change (ΔH) of 176 kJ/mol and an entropy change (ΔS) of 0.285 kJ/(K·mol)—the question arises: at what temperature(s) does this reaction proceed spontaneously?

This comprehensive review aims to dissect this problem thoroughly, exploring the theoretical foundations, deriving necessary equations, and applying them to determine the temperature thresholds for spontaneity. The analysis not only elucidates the thermodynamic principles involved but also provides insights into practical implications for reaction design and control.

Thermodynamic Foundations of Spontaneity

The Gibbs Free Energy: The Criterion for Spontaneity

At the heart of thermodynamic analysis lies the Gibbs free energy change:

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

where:

- ΔG is the Gibbs free energy change,
- ΔH is the enthalpy change,
- ΔS is the entropy change,
- T is the absolute temperature in Kelvin.

A reaction is considered spontaneous when:

$$\Delta G < 0$$

Conversely, non-spontaneous reactions occur when:

$$\Delta G > 0$$

and at equilibrium:

$$\Delta G = 0$$

The temperature at which the reaction shifts from non-spontaneous to spontaneous (or vice versa) is obtained by setting ΔG to zero:

$$0 = \Delta H - T_{\text{crit}} \Delta S$$

which yields the critical temperature (T_{crit}):

$$T_{\text{crit}} = \frac{\Delta H}{\Delta S}$$

This simple relation provides the key to understanding the temperature dependence of reaction spontaneity.

Analyzing the Thermodynamic Data

Given Data:

- Enthalpy change, $\Delta H = 176 \text{ kJ/mol}$
- Entropy change, $\Delta S = 0.285 \text{ kJ/(K}\cdot\text{mol)}$

Note: The units are consistent for the calculation since both are in kJ.

Calculating the Critical Temperature

Applying the formula:

$$T_{\text{crit}} = \frac{\Delta H}{\Delta S}$$

we substitute the given values:

$$T_{\text{crit}} = \frac{176 \text{ kJ/mol}}{0.285 \text{ kJ/(K}\cdot\text{mol)}}$$

Calculating:

$$T_{\text{crit}} \approx \frac{176}{0.285}$$

$$T_{\text{crit}} \approx 617.54 \text{ K}$$

This temperature marks the boundary where the free energy change switches sign.

Interpreting the Results

Spontaneity at Different Temperatures

- For $T < 617.54 \text{ K}$:

Since $\Delta H > 0$ and $\Delta S > 0$, the reaction's spontaneity depends on the temperature. Because ΔH is positive, the reaction is non-spontaneous at low temperatures, where the $T\Delta S$ term isn't sufficient to make ΔG negative. Specifically, for temperatures below T_{crit} :

$$\Delta G = \Delta H - T \Delta S > 0$$

Therefore, the reaction is non-spontaneous at temperatures below approximately 618 K.

- For $T > 617.54 \text{ K}$:

As temperature increases beyond the critical point, the $T\Delta S$ term dominates, rendering ΔG negative:

$$\Delta G < 0$$

Hence, the reaction becomes spontaneous at temperatures above approximately 618 K.

Practical Implications and Contextual Considerations

Understanding the temperature-dependent spontaneity is essential in various industrial and laboratory settings. For reactions with positive ΔH and ΔS , such as the one described, high temperatures favor spontaneity. Conversely, reactions with negative ΔH and ΔS behave differently, often becoming spontaneous at low temperatures.

Key considerations include:

- Reaction Control: Adjusting temperature to optimize yield and rate.
- Energy Efficiency: Recognizing when high temperatures are necessary, which impacts process costs.
- Safety: Managing exothermic reactions that become spontaneous at higher temperatures.

Additional Thermodynamic Factors

While the primary analysis revolves around ΔH and ΔS , real-world reactions are influenced by other factors, such as:

- Pressure: Especially relevant for gaseous reactions.
- Reaction Quotients: Concentrations or partial pressures.
- Kinetics: Spontaneity doesn't imply rapid reaction; activation energy barriers also matter.

In this context, the thermodynamic calculation provides the equilibrium perspective, indicating whether the reaction favors product formation at a given temperature, but kinetic factors determine the rate at which equilibrium is approached.

Limitations and Further Considerations

- Assumption of Constant ΔH and ΔS : The calculations presume that enthalpy and entropy changes are temperature-independent, which is a simplification. In reality, these parameters can vary with temperature.
- Standard State Conditions: The values are typically for standard conditions; deviations may alter the critical temperature.
- Reaction Mechanism: The thermodynamic analysis does not account for pathway-specific factors or activation barriers.

Summary and Conclusions

Based on the thermodynamic data provided:

- The critical temperature (T_{crit}) where the reaction becomes spontaneous is approximately 618 K.
- Below 618 K, the reaction is non-spontaneous.
- Above 618 K, the reaction proceeds spontaneously.

These insights enable chemists and engineers to tailor reaction conditions effectively. For processes requiring spontaneity, operating at temperatures above 618 K ensures thermodynamic favorability. However, practical considerations—such as equipment limitations, energy costs, and safety—must be balanced with thermodynamic predictions.

Final Remarks

This detailed analysis underscores the importance of thermodynamic principles in predicting reaction behavior. While the numerical calculation provides a clear threshold, real-world applications demand integrating these insights with kinetic analysis, process engineering, and safety protocols. As such, understanding the temperature dependence of reaction spontaneity remains a cornerstone in advancing chemical science and industrial practice.

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