

The Rate Constant Of A Reaction Is $4.3 \times 10^3 \text{ s}^{-1}$ At 25°C , And The Activation Energy Is 33.6 kJ/mol . What

The Rate Constant Of A Reaction Is $4.3 \times 10^3 \text{ s}^{-1}$ At 25°C , And The Activation Energy Is 33.6 kJ/mol . What

Understanding the relationship between the rate constant, activation energy, and temperature is fundamental in chemical kinetics. When given specific data such as the rate constant (k) at a certain temperature and the activation energy (E_a), chemists can predict how the reaction rate will change under different conditions, estimate reaction mechanisms, and design processes more efficiently. This article explores the significance of these parameters, the theoretical background, and how to utilize the given data to analyze the reaction's behavior.

Overview of Reaction Kinetics and Rate Constants

What Is the Rate Constant?

The rate constant (k) is a proportionality factor in the rate law expression that relates the reaction rate to the concentrations of reactants. Its units depend on the order of the reaction:

- First-order reactions: s^{-1}
- Second-order reactions: $\text{M}^{-1}\cdot\text{s}^{-1}$
- Zero-order reactions: $\text{M}\cdot\text{s}^{-1}$

In this context, the rate constant is given as $4.3 \times 10^3 \text{ s}^{-1}$, which suggests a first-order process, typical for many reactions involving a single reactant or a rate-determining step with a unimolecular transition state.

What Is Activation Energy?

Activation energy (E_a) is the minimum energy barrier that reactants must overcome for a reaction to proceed. It influences the reaction rate significantly:

- High E_a means slower reaction rates at a given temperature.
- Low E_a indicates faster reactions.

The units of E_a are often expressed in kilojoules per mole (kJ/mol) or calories per mole (cal/mol). In this case, E_a is 33.6 kJ/mol .

Theoretical Background: The Arrhenius Equation

Arrhenius Equation and Its Significance

The Arrhenius equation describes how the rate constant depends on temperature and activation energy:

$$k = A e^{-\frac{E_a}{RT}}$$

Where:

- k = rate constant
- A = pre-exponential factor (frequency of collisions with proper orientation)
- E_a = activation energy (J/mol)
- R = universal gas constant (8.314 J/mol·K)
- T = temperature in Kelvin

This equation indicates that as temperature increases, the exponential term becomes larger, leading to an increase in k .

Understanding the Components

- The pre-exponential factor A accounts for the frequency of collisions and molecular orientation.
- The exponential term reflects the fraction of molecules with enough energy to surpass the activation barrier.

Calculating Reaction Parameters Using Given Data

Given Data Recap

- Rate constant, $k_1 = 4.3 \times 10^3 \text{ s}^{-1}$ at $T_1 = 25^\circ\text{C}$
- Activation energy, $E_a = 33.6 \text{ kJ/mol}$

First, convert temperature to Kelvin:

$$T_1 = 25^\circ\text{C} + 273.15 = 298.15 \text{ K}$$

Estimating the Pre-exponential Factor A

Using the Arrhenius equation:

$$k = A e^{-\frac{E_a}{RT}}$$

Rearranged to solve for A :

$$A = \frac{k}{e^{-\frac{E_a}{RT}}} = k e^{\frac{E_a}{RT}}$$

Calculate A :

$$[A = 4.3 \times 10^3 \times e^{\frac{33,600}{8.314 \times 298.15}}]$$

Calculate the exponent:

$$[\frac{33,600}{8.314 \times 298.15} \approx \frac{33,600}{2478.0} \approx 13.55]$$

Now, compute $(e^{13.55})$:

$$[e^{13.55} \approx \text{exp}(13.55) \approx 7.7 \times 10^5]$$

Finally:

$$[A \approx 4.3 \times 10^3 \times 7.7 \times 10^5 \approx 3.31 \times 10^9 \text{ s}^{-1}]$$

This pre-exponential factor indicates the frequency of successful collisions leading to reaction.

Predicting the Rate Constant at Different Temperatures

Using the Arrhenius Equation to Find (k) at a New Temperature

Suppose we want to find the rate constant at a different temperature, say 50°C (323.15 K). The Arrhenius equation can be rearranged:

$$[\ln \left(\frac{k_2}{k_1} \right) = \frac{E_a}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)]$$

Where:

- (k_1) = known rate constant at (T_1)

- (k_2) = unknown rate constant at (T_2)

Substitute the known values:

$$[\ln \left(\frac{k_2}{4.3 \times 10^3} \right) = \frac{33,600}{8.314} \left(\frac{1}{298.15} - \frac{1}{323.15} \right)]$$

Calculate the right side:

$$[\frac{33,600}{8.314} \approx 4,039.]$$

Calculate the temperature reciprocals:

$$[\frac{1}{298.15} \approx 0.003355, \text{K}^{-1}]$$

$$[\frac{1}{323.15} \approx 0.003094, \text{K}^{-1}]$$

Difference:

$$[0.003355 - 0.003094 = 0.000261, \text{K}^{-1}]$$

Multiply:

$$[4,039 \times 0.000261 \approx 1.055]$$

Exponentiate:

$$[\frac{k_2}{4.3 \times 10^3} = e^{1.055} \approx 2.87]$$

Calculate k_2 :

$$[k_2 \approx 2.87 \times 4.3 \times 10^3 \approx 1.23 \times 10^4, \text{ s}^{-1}]$$

This demonstrates that increasing temperature significantly increases the reaction rate.

Implications for Reaction Dynamics and Design

Understanding Reaction Rates in Practical Contexts

- The reaction accelerates with higher temperatures, consistent with the Arrhenius model.
- Knowledge of k at different temperatures allows for better control of process conditions.

Designing Industrial Processes

- Estimating reaction times based on rate constants.
- Adjusting temperature to optimize yield and efficiency.
- Calculating the energy cost associated with heating or cooling to achieve desired rates.

Additional Considerations and Advanced Applications

Reaction Mechanism Insights

- The activation energy provides clues about the reaction pathway.
- Comparing E_a values across similar reactions can suggest whether a reaction is concerted or involves intermediates.

Limitations of the Arrhenius Model

- Assumes a single dominant energy barrier.
- May not accurately describe reactions with complex mechanisms or multiple steps.
- Temperature dependence of (A) is often neglected but can be significant in some cases.

Extensions and Related Concepts

- Transition State Theory provides a more detailed framework.
- The Eyring Equation offers an alternative approach to analyze temperature dependence.
- Kinetic isotope effects can further elucidate reaction mechanisms.

Summary and Conclusions

- Given the rate constant of $4.3 \times 10^3 \text{ s}^{-1}$ at 25°C and activation energy of 33.6 kJ/mol , one can estimate the pre-exponential factor A , which is approximately $3.31 \times 10^9 \text{ s}^{-1}$.
- Using the Arrhenius equation, we can predict how the reaction rate will change with temperature, as demonstrated with calculations at 50°C .
- Understanding these parameters helps in designing chemical processes, optimizing reaction conditions, and gaining mechanistic insights.
- The exponential relationship between k and T underscores the importance of temperature control in chemical reactions.

By mastering the application of the Arrhenius equation and understanding the significance of activation energy and rate constants, chemists can effectively manipulate reaction conditions to achieve desired outcomes, improve efficiency, and develop safer, more sustainable chemical processes.

Frequently Asked Questions

What is the rate constant (k) of the reaction at 25°C ?

The rate constant is $4.3 \times 10^3 \text{ s}^{-1}$ at 25°C .

What is the activation energy (E_a) of the reaction?

The activation energy is 33.6 kJ/mol .

How does the rate constant change with temperature for this reaction?

The rate constant increases with temperature according to the Arrhenius equation, since E_a is positive.

If the temperature is increased, how would the rate constant change?

The rate constant would increase as temperature increases, due to the exponential dependence in the Arrhenius equation.

What is the significance of the activation energy in this reaction?

Activation energy represents the minimum energy needed for the reactants to convert into products, influencing the reaction rate.

How can the rate constant be used to determine the reaction's rate at 25°C?

The rate constant directly relates to the reaction rate; knowing k allows calculation of the reaction rate when the concentration is known.

What formula relates the rate constant to temperature and activation energy?

The Arrhenius equation: $k = A e^{(-E_a / (RT))}$, where A is the pre-exponential factor, R is the gas constant, and T is temperature in Kelvin.

How would you calculate the rate constant at a different temperature using E_a ?

Use the Arrhenius equation to compare the rate constants at different temperatures by plugging in the values for E_a , R , and T .

Additional Resources

The Rate Constant Of A Reaction Is $4.3 \times 10^3 \text{ s}^{-1}$ At 25°C, And The Activation Energy Is 33.6 kJ/mol. What

Understanding the rate constant and activation energy of a chemical reaction is fundamental in the field of chemical kinetics. These parameters provide critical insights into how quickly a reaction proceeds and the energy barrier that must be overcome for the reaction to occur. In this article, we will explore the significance of the provided data, interpret what it reveals about the reaction's behavior at 25°C, and discuss how temperature influences reaction rates. Additionally, we will analyze the Arrhenius equation's role in connecting the rate constant and activation energy, supported by relevant calculations, and examine real-world applications where such kinetic parameters are pivotal.

Understanding the Rate Constant and Activation Energy

What Is the Rate Constant?

The rate constant (k) is a proportionality factor in the rate law of a chemical reaction. It quantifies the speed at which reactants are converted into products under specific conditions. The units of the rate constant depend on the overall order of the reaction; in this case, the units are s^{-1} , indicating a first-order reaction.

A rate constant of $4.3 \times 10^3 \text{ s}^{-1}$ at 25°C suggests that the reaction proceeds quite rapidly at room temperature, with a high probability of reactant molecules crossing the energy barrier to form products in a very short time frame.

What Is Activation Energy?

Activation energy (E_a) is the minimum energy barrier that reacting molecules must overcome for a successful collision leading to a reaction. It reflects the energy difference between the reactants' energy level and the transition state. A lower E_a generally correlates with a faster reaction at a given temperature.

In this scenario, the activation energy is 33.6 kJ/mol . This relatively moderate value indicates that at room temperature, a significant portion of molecules can surmount this barrier, resulting in the high rate constant observed.

Interpreting the Data: Reaction Rate at 25°C

The given data points to a reaction that is quite rapid at 25°C , which is typical of many biological or industrial reactions designed to proceed swiftly under mild conditions. To understand the implications, let's analyze how the rate constant relates to the reaction's temperature and energy barrier.

Key points:

- High rate constant ($4.3 \times 10^3 \text{ s}^{-1}$): Indicates a fast reaction, with a large number of molecules reacting per second.
- Activation energy (33.6 kJ/mol): Suggests a moderate energy barrier, not too high to hinder the reaction at room temperature.
- Temperature (25°C or 298 K): Standard laboratory conditions, often used as a reference point for kinetic calculations.

This data allows us to evaluate the reaction's potential behavior at different temperatures and predict how modifying conditions could influence the reaction rate.

The Arrhenius Equation: Connecting Rate Constant and Activation Energy

Formulation of the Arrhenius Equation

The Arrhenius equation provides a quantitative relationship between the rate constant (k), temperature (T), and activation energy (E_a):

$$k = A \times e^{-\frac{E_a}{RT}}$$

Where:

- k = rate constant
- A = pre-exponential factor (frequency of collisions with proper orientation)
- E_a = activation energy (J/mol)
- R = universal gas constant (8.314 J/mol·K)
- T = temperature in Kelvin

This equation explains how the rate constant increases with temperature and decreases with higher activation energy.

Calculating the Pre-Exponential Factor (A)

Given:

- $k = 4.3 \times 10^3 \text{ s}^{-1}$
- $E_a = 33.6 \text{ kJ/mol} = 33600 \text{ J/mol}$
- $T = 25^\circ \text{C} = 298 \text{ K}$

Rearranging the Arrhenius equation:

$$A = \frac{k}{e^{-\frac{E_a}{RT}}}$$

Calculating the exponential term:

$$\frac{E_a}{RT} = \frac{33600}{8.314 \times 298} \approx \frac{33600}{2477.772} \approx 13.55$$

Thus:

$$e^{-\frac{E_a}{RT}} = e^{-13.55} \approx 1.3 \times 10^{-6}$$

Now, solving for A:

$$A = \frac{4.3 \times 10^3}{1.3 \times 10^{-6}} \approx 3.31 \times 10^9 \text{ s}^{-1}$$

Interpretation:

The pre-exponential factor (A) is approximately $(3.31 \times 10^9, \text{s}^{-1})$. This value represents the frequency of collisions with the correct orientation and energy for reaction, indicating a highly reactive system with frequent successful collisions.

Predicting Reaction Behavior at Different Temperatures

The Arrhenius equation allows us to estimate the rate constant at temperatures other than 25°C. For example, what would happen to the reaction rate at 40°C (313 K)?

Using the previously calculated A:

$$k_{40^\circ\text{C}} = A \times e^{-\frac{E_a}{RT_{40^\circ\text{C}}}}$$

Calculate:

$$\frac{E_a}{RT_{40^\circ\text{C}}} = \frac{33600}{8.314 \times 313} \approx \frac{33600}{2604.98} \approx 12.89$$

$$e^{-\frac{E_a}{RT_{40^\circ\text{C}}}} = e^{-12.89} \approx 2.55 \times 10^{-6}$$

Therefore:

$$k_{40^\circ\text{C}} = 3.31 \times 10^9 \times 2.55 \times 10^{-6} \approx 8.45 \times 10^3, \text{s}^{-1}$$

Implication:

At 40°C, the rate constant increases to approximately $8.45 \times 10^3 \text{s}^{-1}$, nearly doubling the reaction speed at 25°C. This demonstrates the sensitivity of the reaction rate to temperature changes, aligning with the principles of Arrhenius kinetics.

Features and Limitations

Features:

- Predictive Power: The Arrhenius equation allows for the estimation of reaction rates at various temperatures.
- Insight into Reaction Mechanism: Activation energy provides clues about the complexity and energy barriers involved.
- Design of Industrial Processes: Knowledge of kinetic parameters helps optimize reaction conditions for efficiency.

Limitations:

- Assumption of a Single Activation Energy: Many reactions involve multiple steps with different E_a values, complicating the analysis.
- Pre-exponential Factor Variability: A assumes a constant collision frequency, which may vary with temperature and other factors.
- Neglect of External Factors: Catalysts, pressure, and solvent effects are not directly accounted for.

Applications of Kinetic Data in Real-World Scenarios

Understanding the rate constant and activation energy is vital across numerous fields:

- Pharmaceutical Development: Optimizing reaction conditions for drug synthesis.
- Industrial Catalysis: Designing catalysts that lower activation energy and increase production efficiency.
- Environmental Chemistry: Modeling pollutant degradation rates under various conditions.
- Biochemistry: Understanding enzyme kinetics where activation energy influences metabolic pathways.

Conclusion

The provided data on the rate constant and activation energy offers a window into the reaction's kinetic profile at 25°C. The high rate constant reflects a reaction that proceeds rapidly under ambient conditions, with a moderate activation energy facilitating this speed. By applying the Arrhenius equation, we can further analyze how temperature influences the rate, enabling predictions and optimizations relevant to scientific research and industrial applications. While the parameters offer valuable insights, it's essential to consider the inherent assumptions and external factors that may affect reaction kinetics. Overall, these kinetic parameters are foundational tools for chemists seeking to understand, control, and harness chemical reactions effectively.

Key Takeaways:

- The rate constant of $4.3 \times 10^3 \text{ s}^{-1}$ indicates a fast reaction at 25°C.
- Activation energy of 33.6 kJ/mol is moderate, facilitating reaction progress at room temperature.
- Calculations show how temperature influences the rate constant via the Arrhenius equation.
- Practical applications span industries and scientific disciplines, emphasizing the importance of kinetic data.

End of Article

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