Kinetic and Arrhenius Analysis of a Chemical Reaction Using Python

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Tools Used: Python (NumPy, Matplotlib, SciPy)

Abstract

The kinetics of a chemical reaction were analyzed using integrated rate laws and Arrhenius theory implemented through Python-based data analysis. First-order kinetics were confirmed using ln[A] versus time plots with high linearity ($R^2 \approx 0.99995$). The Arrhenius plot of ln k versus 1/T showed excellent agreement with theory ($R^2 \approx 0.99901$), yielding an activation energy of approximately 60.3 kJ/mol. The study demonstrates the effectiveness of computational tools in extracting reliable kinetic parameters from experimental data.

1. Introduction and Theory

Chemical kinetics examines reaction rates and their dependence on concentration and temperature. For a first-order reaction, the integrated rate law ln[A] = ln[A■] – kt predicts a linear relationship between ln[A] and time. Temperature dependence of rate constants is described by the Arrhenius equation, ln k = ln A – (Ea/R)(1/T), allowing determination of activation energy.

2. Methodology

Experimental concentration–time data were analyzed using Python. Linear regression was applied to ln[A] versus time plots to determine reaction order and rate constants. Arrhenius analysis was performed by plotting ln k against 1/T. Statistical reliability was evaluated using R^2 values.

3. Results

The ln[A] versus time plot showed strong linearity ($R^2 \approx 0.99995$), confirming first-order kinetics. Arrhenius analysis produced a linear ln k versus 1/T plot with $R^2 \approx 0.99901$. The activation energy was calculated to be approximately 60.3 kJ/mol.

4. Discussion

The results indicate that the reaction follows a single-step first-order mechanism. The negative slope of the Arrhenius plot reflects the inverse relationship between ln k and 1/T. High R^2 values confirm the suitability of the selected kinetic and Arrhenius models.

5. Error Analysis and Assumptions

Potential sources of error include temperature measurement uncertainty and concentration measurement limitations. The analysis assumes a single rate-determining step and negligible side reactions.

6. Conclusion

This study successfully applied computational methods to determine reaction kinetics and activation energy. The integration of physical chemistry theory with Python-based analysis demonstrates a reliable approach for quantitative kinetic studies.

7. Skills and Tools Demonstrated

Chemical kinetics, Arrhenius analysis, data regression, scientific visualization, Python programming, and critical interpretation of physical chemistry data.