Reaction order and graphing:

zero order reaction (A -> B) with a rate constant k

The integrated rate equation for a zero order reaction:

\[ A(0) - A(t) = k \cdot t \]

Rearrage

\[ A(t) = -k \cdot t + A(0) \]

Plot of [A] vs t has:
- slope of -k
- y intercept of A(0).

Variables and equations

\[ k := 1.5 \times 10^{-3} \text{ mole} \cdot \text{liter}^{-1} \cdot \text{sec}^{-1} \]
- Rate constant

\[ t := 0 \text{ sec}, 1 \text{ sec}..1000 \text{ sec} \]
- Range of times to plot

\[ A_0 := 3 \text{ mole} \cdot \text{liter}^{-1} \]
- Initial concentration

\[ A(t) := -k \cdot t + A_0 \]
- Concentration of A at time t

zero order reaction:
Zero order kinetics plot

\[ \frac{A(t)}{\text{mole} \cdot \text{liter}^{-1}} \]

\[ t \quad \text{sec} \]
First order reaction (A -> B) with a rate constant k

The integrated rate equation for a first order reaction:

\[
\ln \left( \frac{A(t)}{A(0)} \right) = -k \cdot t
\]

Rearrange

\[
\ln(A(t)) = -k \cdot t + \ln(A(0))
\]

Plot of ln [A] vs t has slope of -k and y intercept of -\ln(A(0)).

\[
A(t) = e^{-k \cdot t}
\]

Rearranged to give the concentration of A at time t.

Variables and equations

\[
k := 5.0 \cdot 10^{-3} \cdot \text{sec}^{-1}
\]

Rate constant

\[
A(t) := e^{-k \cdot t + \ln \left( \frac{A_0}{\text{mole} \cdot \text{liter}^{-1}} \right)}
\]

Concentration of A at time t for a first order reaction:
First order kinetics plot

Logarithmic first order kinetics plot
Second order reaction (A -> B) with a rate constant k

The integrated rate equation for a second order reaction:

\[
\frac{1}{A(t)} - \frac{1}{A(0)} = k \cdot t
\]

Rearrange

\[
\frac{1}{A(t)} = k \cdot t + \frac{1}{A(0)}
\]

Plot of \((1/[A])\) vs t has slope of k

y intercept of \((1/A(0))\)

\[
A(t) = \frac{1}{k \cdot t + \frac{1}{A(0)}}
\]

Rearranged to give the concentration of A at time t.

Variables and equations

\[
k := 4 \cdot \text{liter} \cdot \text{mole}^{-1} \cdot \text{sec}^{-1}
\]

Rate constant

\[
A(t) := \frac{1}{k \cdot t + \frac{1}{A_0 \cdot \text{liter/mole}}}
\]

Concentration of A at time t for a second order reaction:
Second order kinetics plot

$A(t)$

$t \text{ (sec)}$

1/conc second order kinetics plot

$\frac{1}{A(t)}$

$t \text{ (sec)}$
Graphing the Arrhenius equation, calculate activation energy and the pre-exponential factor from:

<table>
<thead>
<tr>
<th>Temp (K)</th>
<th>Rate Constant (sec⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tᵢ</td>
<td>kᵢ</td>
</tr>
<tr>
<td>273</td>
<td>7.78 · 10⁻⁷</td>
</tr>
<tr>
<td>298</td>
<td>3.46 · 10⁻⁵</td>
</tr>
<tr>
<td>318</td>
<td>4.98 · 10⁻⁴</td>
</tr>
<tr>
<td>328</td>
<td>1.50 · 10⁻³</td>
</tr>
<tr>
<td>338</td>
<td>4.87 · 10⁻³</td>
</tr>
</tbody>
</table>

Data Set  \( N := 5 \)  \( i := 0, 1 \ldots N - 1 \)  \( R := 8.314510 \text{ joule} \cdot \text{K}^{-1} \cdot \text{mole}^{-1} \)
Regression Analysis:

\[ x_i := \frac{1}{T_i} \]

\[ y_i := \ln(k_i) \]

Calculation of line:

Slope: \[ m := \text{slope}(x, y) \quad m = -1.239 \cdot 10^4 \]

Intercept: \[ b := \text{intercept}(x, y) \quad b = 31.321 \]

Calculation of Activation Energy and Collision Frequency

\[ E_a := -m \cdot R \cdot K \quad E_a = 1.03 \cdot 10^5 \text{ joule mole}^{-1} \]

\[ A := e^b \cdot \text{sec}^{-1} \quad A = 4.005 \cdot 10^{13} \text{ sec}^{-1} \]