Reaction order and graphing:

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

The integrated rate equation for a zero order reaction:

$$A(0) - A(t) = k \cdot t$$

Rearange

$$A(t) = -k \cdot t + A(0)$$

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

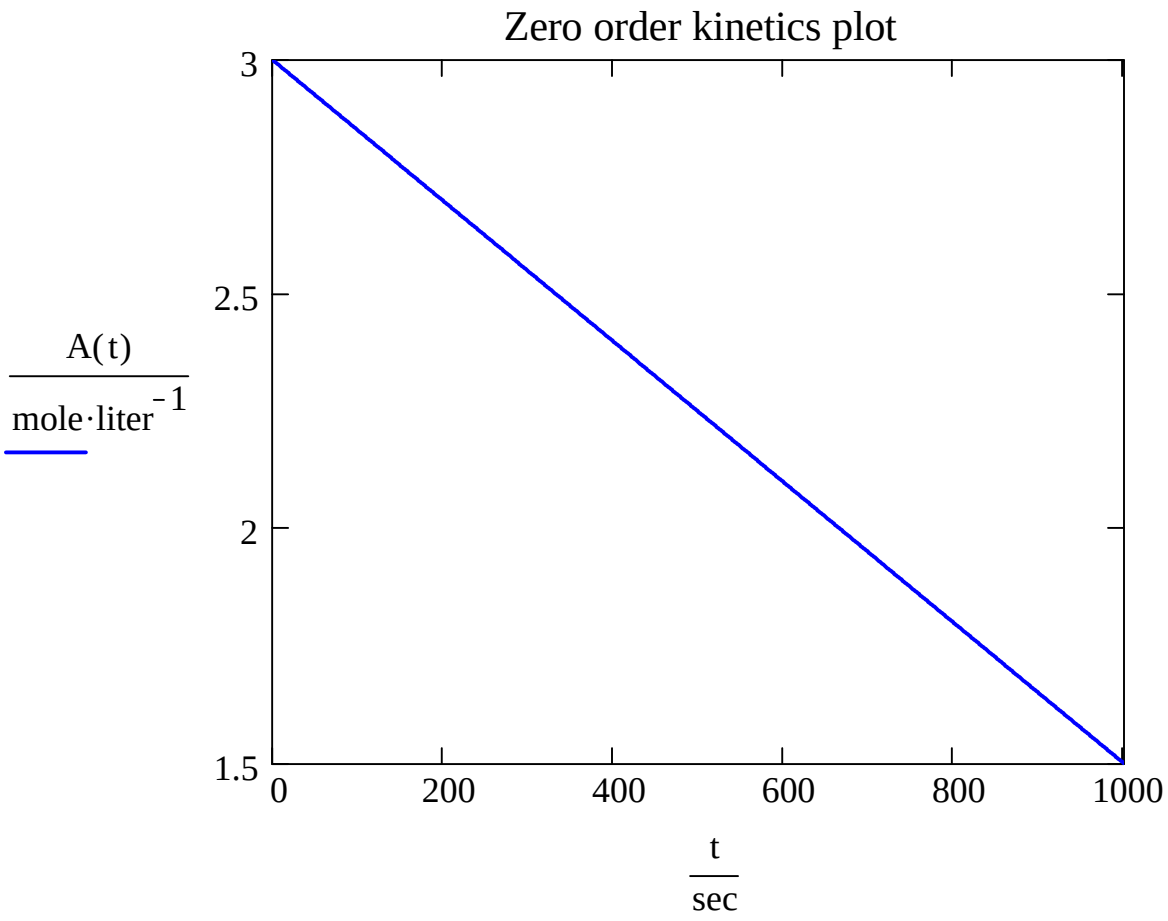
Variables and equations

$k := 1.5 \cdot 10^{-3} \cdot mole \cdot liter^{-1} \cdot sec^{-1}$ Rate constant

$t := 0 \cdot sec, 1 \cdot sec .. 1000 \cdot sec$ Range of times to plot

$A_0 := 3 \cdot mole \cdot liter^{-1}$ Initial concentration

$A(t) := -k \cdot t + A_0$ Concentration of A at time t
zero order reaction:


Zero order kinetics plot
A(t)
mole·liter^-1
3
2.5
2
1.5
0
200
400
600
800
1000
t
sec

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

The integrated rate equation for a first order reaction:

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

Rearange

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

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

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

Rearanged to give the concentration of A at time t.

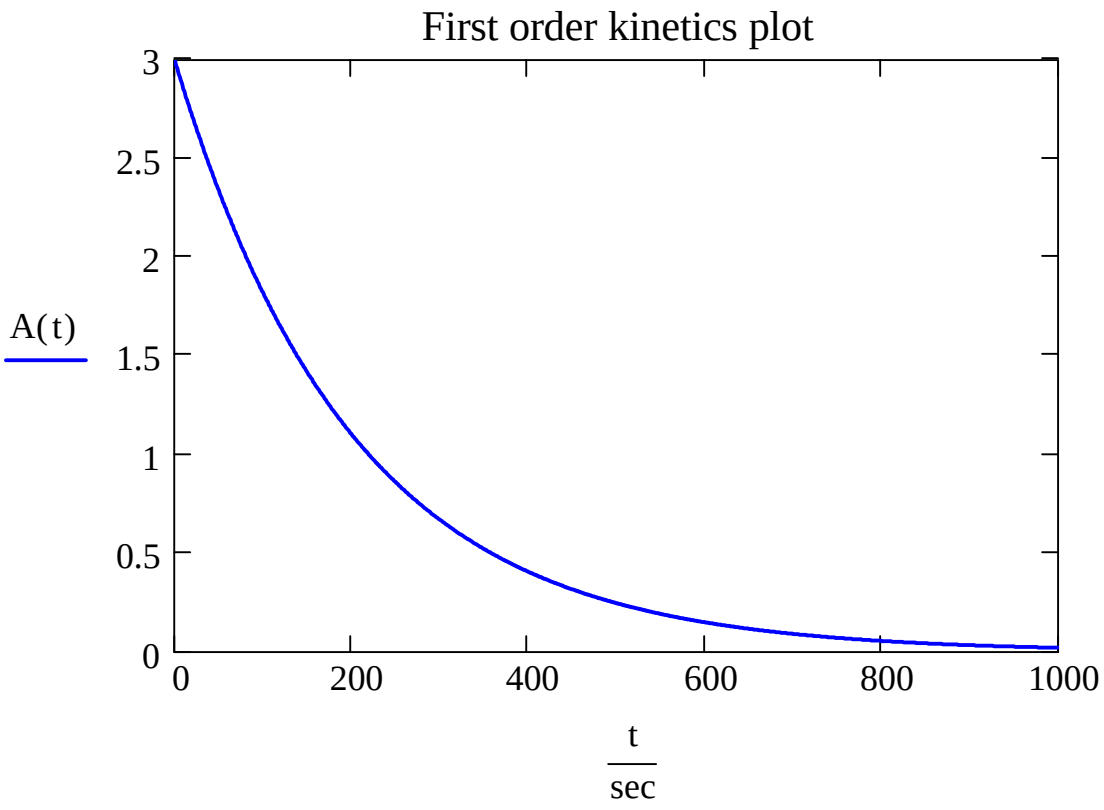
Variables and equations

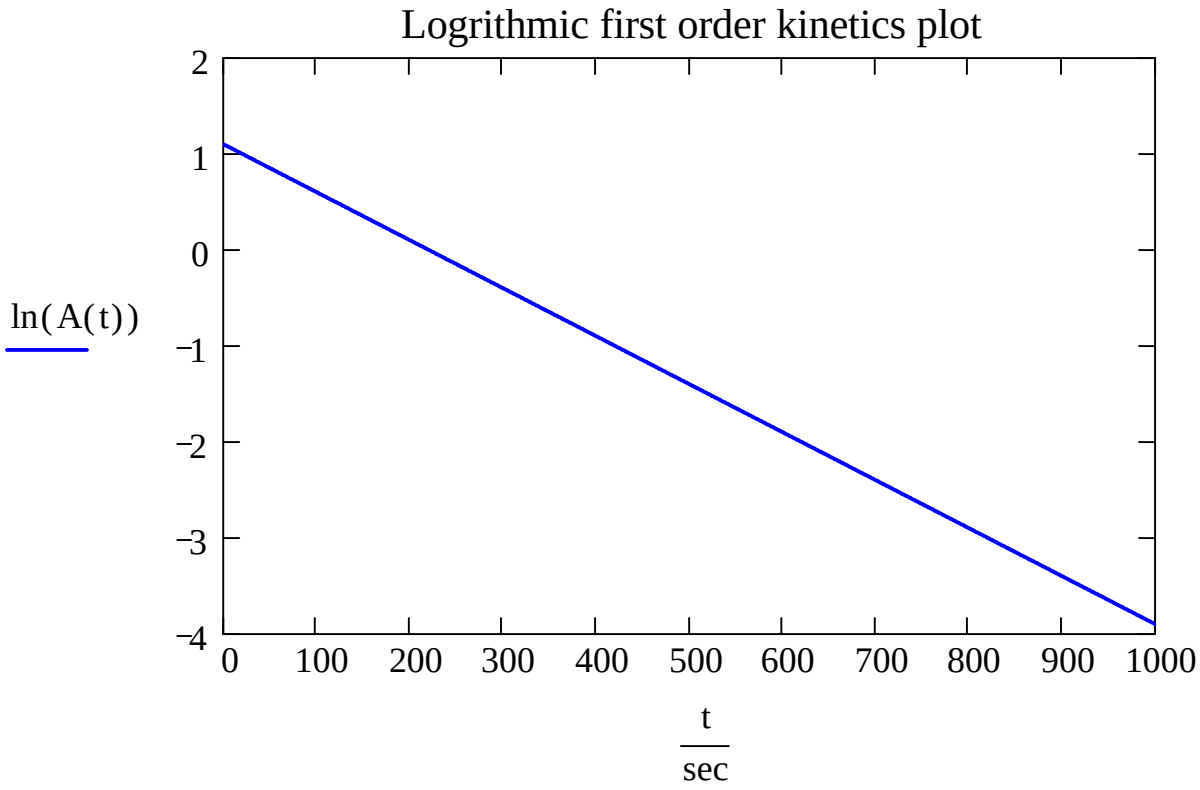
$$k := 5.0 \cdot 10^{-3} \cdot \text{sec}^{-1}$$

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
A(t)
3
2.5
2
1.5
1
0.5
0
0
200
400
600
800
1000
t
sec


Logrithmic first order kinetics plot
ln(A(t))
2
1
0
−1
−2
−3
−4
0
100
200
300
400
500
600
700
800
900
1000
t
sec

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

The integrated rate equation for a second order reaction:

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

Rearange

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

Plot of (1/[A]) vs t has
slope of k
y intercept of (1/A(0))

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

Rearanged to give the concentration of A at time t.

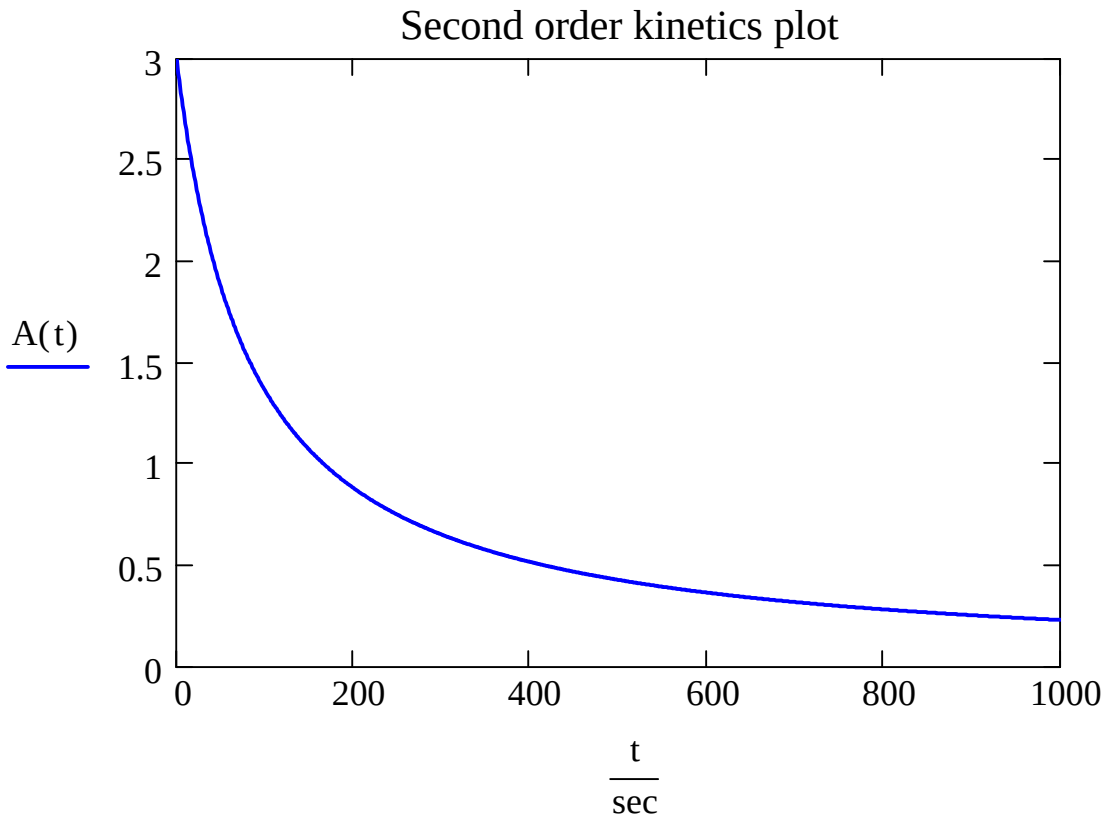
Variables and equations

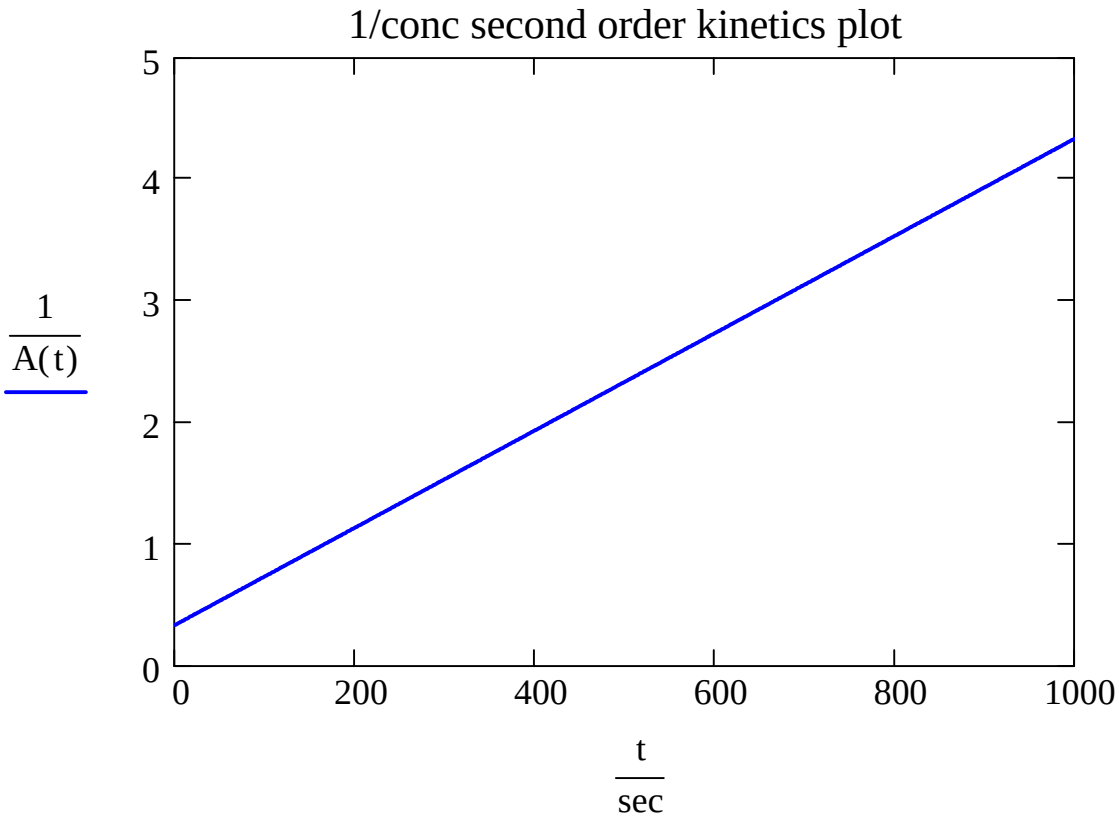
$$k := 4 \cdot \text{liter} \cdot \text{mole}^{-1} \cdot \text{sec}^{-1}$$

Rate constant

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

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


Second order kinetics plot
A(t)
3
2.5
2
1.5
1
0.5
0
0
200
400
600
800
1000
t
sec


1/conc second order kinetics plot
1
A(t)
5
4
3
2
1
0
0
200
400
600
800
1000
t
sec

Graphing the Ahrrenius equation,
Calcuate activation energy and the pre-exponental factor from:

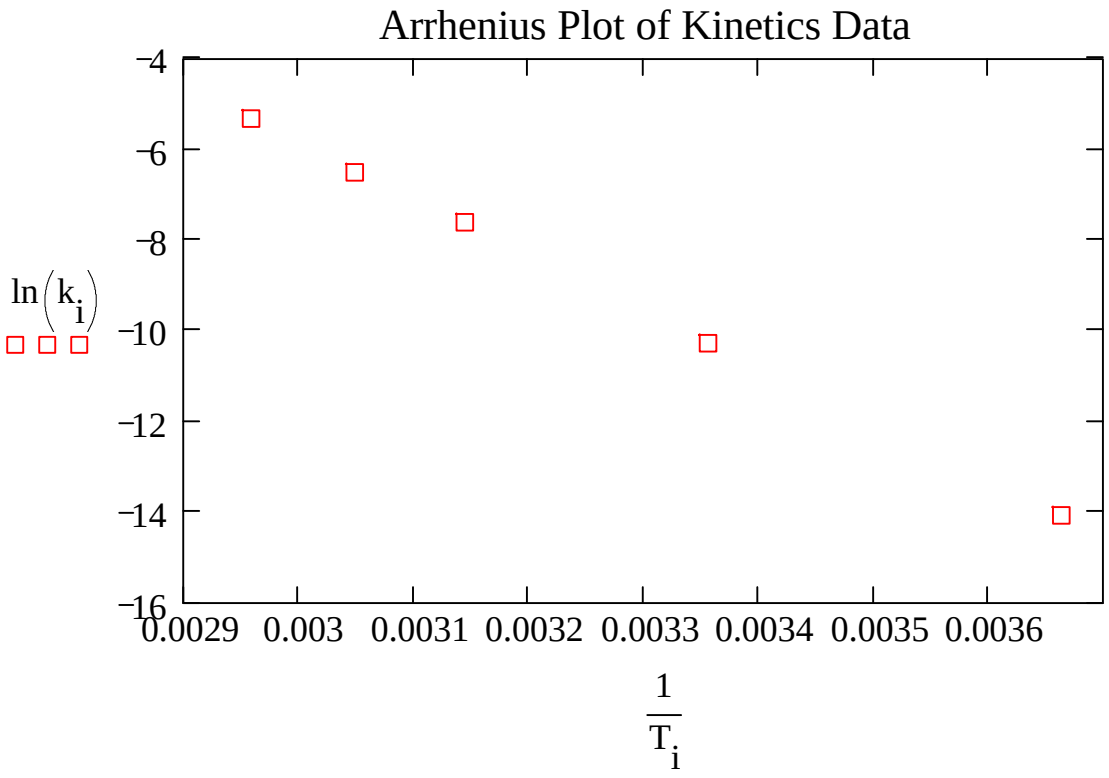
Data Set $N := 5$ $i := 0, 1 .. N - 1$ $R := 8.314510 \cdot joule \cdot K^{-1} \cdot mole^{-1}$

Temp (K) $T_i :=$

273
298
318
328
338

Rate Constant (sec-1) $k_i :=$

$7.78 \cdot 10^{-7}$
$3.46 \cdot 10^{-5}$
$4.98 \cdot 10^{-4}$
$1.50 \cdot 10^{-3}$
$4.87 \cdot 10^{-3}$



Regression Analysis:

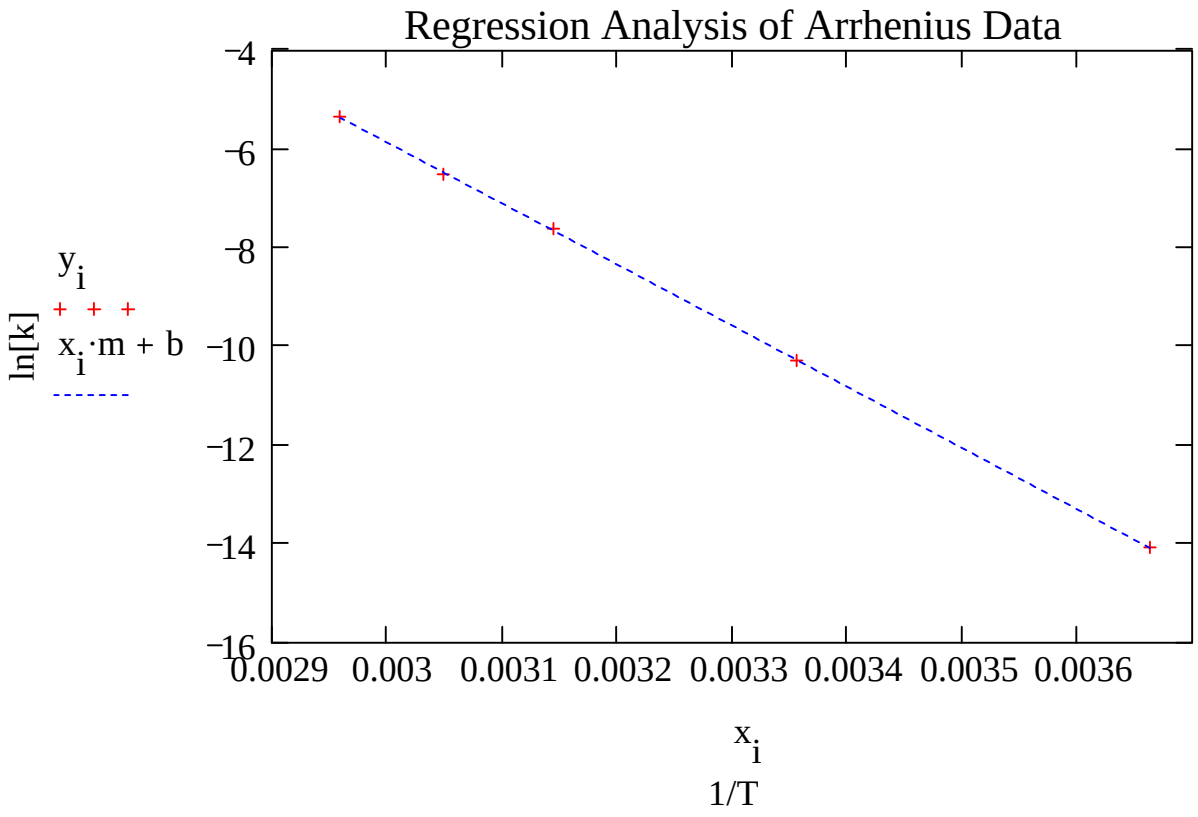
x axis $x_i := \frac{1}{T_i}$

y axis $y_i := \ln(k_i)$

Calculation of line:

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

Intercept: $b := \text{intercept}(x, y)$ $b = 31.321$



Calculation of Activation Energy and Collision Frequency

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

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