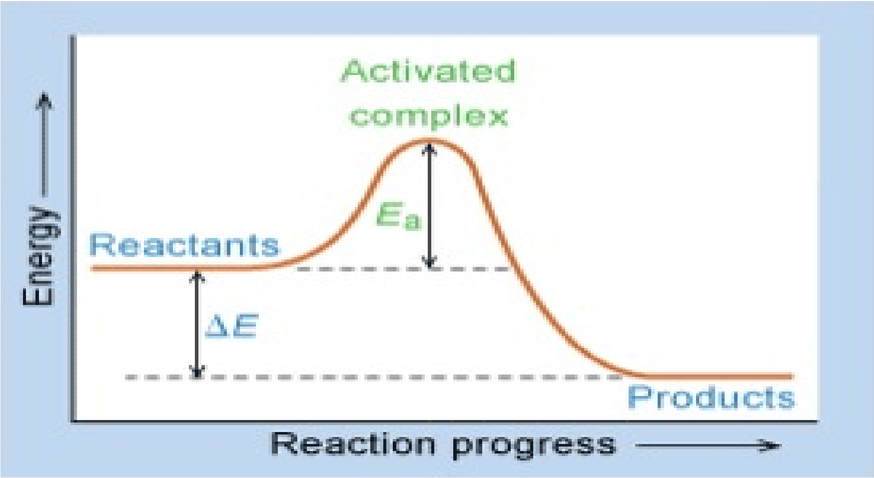
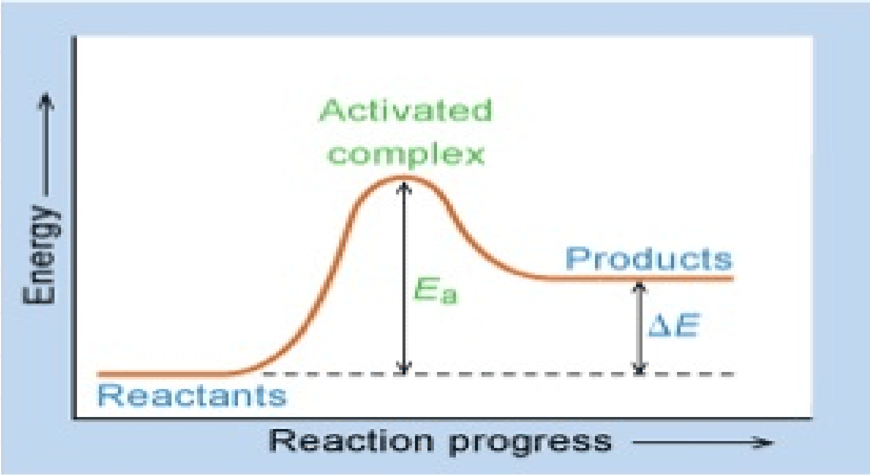
14.5 Activation Energy and Temperature

Reaction Coordinate Diagrams





E_a = Activation Energy

$\Delta E = E_{PRODUCTS} - E_{REACTANTS}$
< 0
Exothermic

$\Delta E = E_{PRODUCTS} - E_{REACTANTS}$
> 0
Endo thermic

14.5 Activation Energy and Temperature

The Arrhenius Equation

$$k = Ae^{-\frac{E_a}{RT}}$$

k : Rate constant.
A : Frequency factor.
E_a : Activation Energy.
R : Ideal Gas Constant.
T : Temperature in K.

A : Measure of the number of collisions that take place with the correct orientation.

$e^{-\frac{E_a}{RT}}$: Fraction of the collisions that occur with sufficient energy to overcome E_a.

a) $E_a \uparrow$, then $e^{-\frac{E_a}{RT}} \downarrow$, $k \downarrow$

b) $E_a \downarrow$, then $e^{-\frac{E_a}{RT}} \uparrow$, $k \uparrow$

$$k_1 = Ae^{-\frac{E_a}{RT_1}} \quad ; \quad k_2 = Ae^{-\frac{E_a}{RT_2}}$$

$$\ln k_1 = \ln(Ae^{-\frac{E_a}{RT_1}}) \quad ; \quad \ln k_2 = \ln(Ae^{-\frac{E_a}{RT_2}})$$

$$\ln k_2 - \ln k_1 = \ln A + \ln e^{-\frac{E_a}{RT_2}} - \ln A - \ln e^{-\frac{E_a}{RT_1}}$$

$$\ln k_2 - \ln k_1 = -\frac{E_a}{RT_2} - \left(-\frac{E_a}{RT_1}\right)$$

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

14.5 Activation Energy and Temperature

The Arrhenius Equation

The **activation energy** for the gas phase decomposition of acetic anhydride is 144 kJ/mol.

$$(CH_3CO)_2O = CH_2{=}C{=}O + CH_3COOH$$

The **rate constant** for this reaction is $6.02\times10^{-4}\ s^{-1}$ at 495 K. What is the **rate constant** at 531 K?

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

$E_a = 144{,}000\ J$ (Remember, R is in J)

$T_1 = 495\ K$ $\quad T_2 = 531\ K$

$k_1 = 6.02\times10^{-4}$ $\quad k_2 = ?$

$R = 8.314\ J.mol^{-1}.K^{-1}$

$$\ln\frac{k_2}{6.02\times10^{-4}} = -\frac{144{,}000}{8.314}\left(\frac{1}{531}-\frac{1}{495}\right)$$

$$\ln k_2 - \ln(6.02\times10^{-4}) = -17320.2\,(-1.3696\times10^{-4})$$

$$\ln k_2 + 7.4152 = 2.3722$$

$$\ln k_2 = 2.3722 - 7.4152$$

$$\ln k_2 = -5.043$$

$$k_2 = 6.45\times10^{-3}\ s^{-1}$$

14.5 Activation Energy and Temperature

Graphical Determination of Ea

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

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

$$\ln k = -\frac{E_a}{RT} + \ln A$$

$$\ln k = -\frac{E_a}{R}\left(\frac{1}{T}\right) + \ln A$$

$$y = m x + c$$

$\ln k$ vs $1/T$ plot, slope $= -\frac{E_a}{R}$

The Arrhenius Equation

Question 1 of 3

The rate of the reaction

$$N_2O_5\,(g) \longrightarrow 2\,NO_2\,(g) + \tfrac{1}{2}O_2\,(g)$$

is measured at different temperatures, with the following rate constants, k, determined:

Temperature, K	k, s^{-1}
298	3.46×10^{-5}
328	1.5×10^{-3}
358	3.34×10^{-2}
378	0.21

What is the activation energy, E_a, for this reaction in units of kilojoules?

Submit

k
ln k
1/k

T   ln T   1/T

Least Squares Analysis

Enter a response, then press **SUBMIT**.

kJ

Plot

Clear

14.5 Activation Energy and Temperature

Graphical Determination of Ea

Slope $= -1.23 \times 10^4$

$-\frac{E_a}{R} = -1.23 \times 10^4$

$-E_a = -1.23 \times 10^4 (8.314)$

$E_a = 1.23 \times 10^4 (8.314)$

$= 1.02 \times 10^5 \text{ J.mol}^{-1}$

OR

102 kJ.mol^{-1}

The Arrhenius Equation

Question 1 of 3

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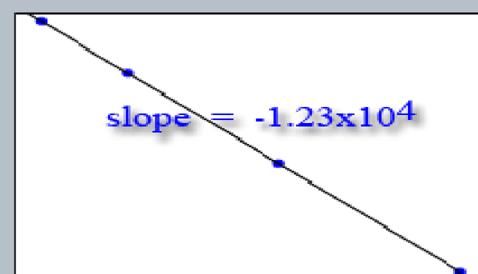
Submit

○ k
◉ ln k
○ 1/k



○ T ○ ln T ◉ 1/T

☑ Least Squares Analysis

Enter a response, then press **SUBMIT**.

102 kJ

Plot

Clear