An Interdisciplinary Study of Chemical Reactions

Connecting Chemistry, Mathematics, and Python

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- Energy and Chemical Reactions
- Thermodynamics in Chemical Reactions
- Chemical Kinetics

The state of a system comes from knowing quantitative properties of it: velocity, position, temperature, mass, etc.

Figure: A comet moving through space

The system changes when these quantities evolve over time. To study this evolution we can consider two different points of view:

- Newton's 2nd law:

$$\vec{F} = m\vec{a}$$

Work is a measure of the '*degree*' of change of a system do to an external force, by considering the change in **position**:

$$W = \vec{F} \cdot \Delta\vec{x}$$

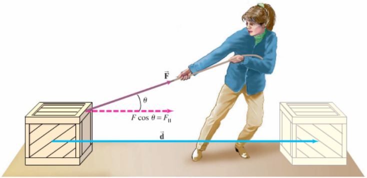


Figure: Work[1]

[1] Douglas C. Giancoli. *Physics. principles with applications*. 2004. Chap. 6, p. 136

- **Energy**:

$$K(v) = \frac{1}{2}mv^2 \quad \text{(Kinetic energy)}$$

$$U(x) = \left\{ mgx, \frac{1}{2}kx^2, \frac{kq_1q_2}{x} \right\} \quad \text{(Potential energy)}$$

$$E(m, T, P, V) = \text{Internal Energy}^{[2]}$$

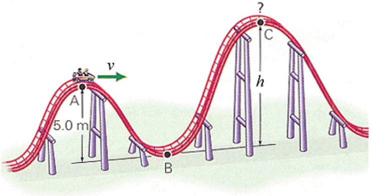
This leads to two powerful principles:

- Energy is **conserved.**
- The energy of a system can change through work or **heat**

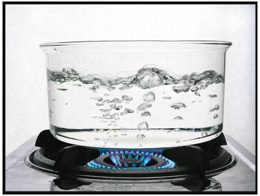
$$\Delta E = W + q \tag{1}$$

This allows us to analyze physical systems by comparing their energy states—often with fewer calculations and more physical insight.

Mechanical Energy: $E(v, x) = K(v) + U(x)$



Internal Energy: $E(m, T, P, V)$



[2] Theodore L. Brown, ed. *Chemistry. The central science*. 13. ed. 2015. Chap. 5, p. 166

Steam Locomotive

Rocket Launch

Both systems convert internal energy into motion — via matter transformation.

$$E(m, T, P, V) \to E(x, v)$$

Chemistry studies the **transformation of matter** due to:

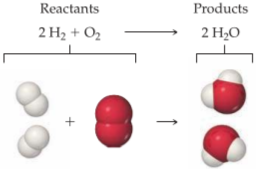
- Change in the physical state (e.g., melting, vaporization)

$$H_2O\,(l) + \text{Energy} \to H_2O\,(g)$$

- Change in composition (chemical reactions)

$$2\,H_2(l) + O_2(l) \longrightarrow 2\,H_2O\,(g) + \text{Energy}$$

A **chemical reaction** can be defined as the transformation of one or more substances into different substances, and can be analyzed qualitatively, quantitatively, or both.



Quantification of changes in mass, and/or temperature

To represent chemical reaction a chemical equation is commonly used:

$$\mathrm{aA\,(g) + bB((l) \; \rightarrow cC\,(s) + dD\,(g)}$$

This indicates the substances that are being transformed (Reactants:left-side) and the new obtained substances (Products:right-side).

1. Chemical Reaction must be balanced (conservation of matter) for that we use a,b,c,d-(stoichiometric coefficients)
2. The physical state must be indicated (l,s,g,aq)

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1. **Write the unbalanced equation.**
   List all reactants and products using correct chemical formulas.
2. **List the number of atoms of each element.**
   Count atoms for each element on both sides.

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Balancing Chemical Equations:

1. **Write the unbalanced equation.**
   List all reactants and products using correct chemical formulas.
2. **List the number of atoms of each element.**
   Count atoms for each element on both sides.
3. **Start balancing with the most complex molecule.**
   Begin with compounds containing the most elements; leave free elements (like O_2 or H_2) for last.
4. **Balance one element at a time using coefficients.**
   Never change subscripts; only adjust coefficients.

   Balance hydrogen and oxygen last.
   These are often involved in multiple compounds.

   Check your work.
   Make sure atom counts are equal on both sides for all elements.

Fraction coefficients can be used to help the balancing process but is recommended that all coefficients must be whole numbers in the final balanced chemical equation.

Example-1:

$$CH_4(g) + O_2(g) \quad \rightarrow \quad CO_2(g) + H_2O\,(g)$$

Try:

Example-2:

$$Na\,(s) + H_2O\,(l) \quad \rightarrow \quad NaOH\,(aq) + H_2(g)$$

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$$CH_4(g) + O_2(g) \rightarrow CO_2(g) + H_2O(g)$$

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Example-2:

$$Na(s) + H_2O(l) \rightarrow NaOH(aq) + H_2(g)$$

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\end{aligned}
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Example-2:

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Na(s) + H_2O(l) \rightarrow NaOH(aq) + H_2(g)
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Example-2:

$$
\begin{aligned}
Na(s) + H_2O(l) &\rightarrow NaOH(aq) + H_2(g) \\
Na(s) + H_2O(l) &\rightarrow NaOH(aq) + {}^1/_2H_2(g)
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Example-2:

$$Na(s) + H_2O(l) \rightarrow NaOH(aq) + H_2(g)$$
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Example-2:

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Try:

$$CH_4(g) + Br_2(l) \rightarrow CBr_4(s) + HBr(g)$$

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Example-2:

$$Na(s) + H_2O(l) \rightarrow NaOH(aq) + H_2(g)$$
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Try:

$$CH_4(g) + Br_2(l) \rightarrow CBr_4(s) + HBr(g)$$
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CH_4(g) + 2O_2(g) &\rightarrow CO_2(g) + 2H_2O(g)
\end{aligned}
$$

Example-2:

$$
\begin{aligned}
Na(s) + H_2O(l) &\rightarrow NaOH(aq) + H_2(g) \\
Na(s) + H_2O(l) &\rightarrow NaOH(aq) + 1/2H_2(g) \\
2Na(s) + 2H_2O(l) &\rightarrow 2NaOH(aq) + H_2(g)
\end{aligned}
$$

Try:

$$
\begin{aligned}
CH_4(g) + Br_2(l) &\rightarrow CBr_4(s) + HBr(g) \\
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\end{aligned}$$

Example-2:

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Na(s) + H_2O(l) &\rightarrow NaOH(aq) + H_2(g) \\
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$$O_2(g) + NO(g) \rightarrow NO_2(g)$$

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Example-2:

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Example-2:

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Try:

$$\begin{aligned} O_2(g) + NO(g) &\rightarrow NO_2(g) \\ {}^1\!/\!_2O_2(g) + NO(g) &\rightarrow NO_2(g) \\ O_2(g) + 2NO(g) &\rightarrow 2NO_2(g) \end{aligned}$$

We can balance the reaction algebraically by assigning variables to each coefficient:

$$a\,Fe + b\,O_2 \rightarrow c\,Fe_2O_3$$

From element counts:

$$\begin{aligned} &\text{Fe:} \quad a = 2c \\ &\text{O:} \quad 2b = 3c \end{aligned}$$

Letting $c = 1$ (a free variable):

$$a = 2, \quad b = \frac{3}{2}$$

Multiply all coefficients by 2 to eliminate the fraction:

$$4\,Fe + 3\,O_2 \longrightarrow 2\,Fe_2O_3$$

Try:

$$Al(s) + HCl(aq) \quad \rightarrow \quad AlCl_3(aq) + H_2(g)$$

Multiply all coefficients by 2 to eliminate the fraction:

$$4\,\mathrm{Fe} + 3\,\mathrm{O_2} \longrightarrow 2\,\mathrm{Fe_2O_3}$$

Try:

$$\begin{aligned} \mathrm{Al(s)} + \mathrm{HCl(aq)} &\rightarrow \mathrm{AlCl_3(aq)} + \mathrm{H_2(g)} \\ x\,\mathrm{Al(s)} + y\,\mathrm{HCl(aq)} &\rightarrow a\,\mathrm{AlCl_3(aq)} + b\,\mathrm{H_2(g)} \end{aligned}$$

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From atom counts:

$$\mathrm{Al}: \;\; x = a, \;\; \mathrm{H}: \;\; y = 2b, \;\; \mathrm{Cl}: \;\; y = 3a$$

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So, $0 = 3a - 2b \to b = (3/2)a$, then

$$x = a, \;\; y = 3a, \;\; b = (3/2)a$$

Letting $a = 1$ we get

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Letting $a = 1$ we get

$$\begin{aligned} \mathrm{Al(s)} + 3\mathrm{HCl(aq)} &\rightarrow \mathrm{AlCl_3(aq)} + 3/2\mathrm{H_2(g)} \\ 2\mathrm{Al(s)} + 6\mathrm{HCl(aq)} &\rightarrow 2\mathrm{AlCl_3(aq)} + 3\mathrm{H_2(g)} \end{aligned}$$

Major Types of Chemical Reactions

Reaction Type	General Form	Example	Description
Combination (Synthesis)	$A + B \rightarrow C$	$N_2(g) + 3\,H_2(g) \rightarrow {}_2NH_3(g)$	Two or more substances combine to form one product.
Decomposition	$C \rightarrow A + B$	$CaCO_3(s) \rightarrow CaO\,(s) + CO_2(g)$	A single compound breaks down into simpler substances.
Combustion	$\text{Fuel} + O_2 \rightarrow \text{Oxides} + \text{Energy}$	$CH_4(g) + 2\,O_2(g) \rightarrow CO_2(g) + 2\,H_2O\,(g)$	A substance reacts with O_2, releasing heat and light. Hydrocarbons yield CO_2 and H_2O.
Single Replacement	$A + BC \rightarrow AC + B$	$Zn\,(s) + HCl(aq) \rightarrow ZnCl_2(aq) + H_2(g)$	One element replaces another in a compound.
Double Replacement	$AB + CD \rightarrow AD + CB$	$AgNO_3(aq) + NaCl(aq) \rightarrow AgCl\,(s) + NaNO_3(aq)$	Ions are exchanged between two compounds; often forms a precipitate, gas, or water.

Why?, How? **Chemical Reactions happen.**

To answer this question we go to the basics, why the state of a system changes?

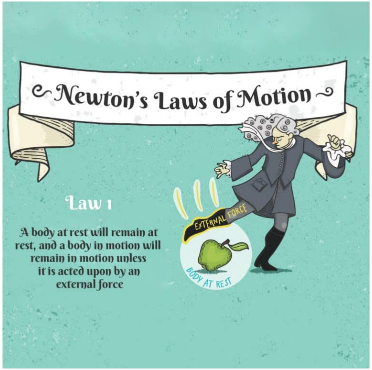

Figure: Newton's 1st Law[3]

[3] Smore Science Staff. *Newton's Laws*. Accessed: 2025-05-22. 2022. URL: https://www.smorescience.com/newtons-laws-of-motion-with-examples/

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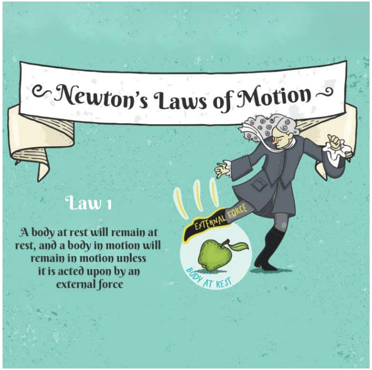

Figure: Newton's 1st Law[3]

$$\begin{array}{ccccc} \vec{F} & \rightarrow & W & \rightarrow & \Delta E \quad \text{(Not necessarily)} \\ \Delta E & \leftarrow & W & \leftarrow & \vec{F} \quad \text{(Necessarily)} \end{array}$$

If a chemical reaction happen, the state of the substance changes, hence there are internal forces making the change possible. (This is the Why?)

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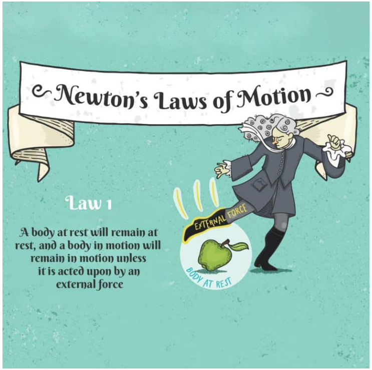

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$$\downarrow$$

The occurrence of **chemical reactions** is analyzed from the perspective of **energy changes** between reactants and products.

$$\Delta E_{\text{reaction}} = E_{\text{products}} - E_{\text{reactants}}$$

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The study of energy and its transformations is known as **thermodynamics** (Greek: thérme-, "heat"; dy'namis, "power"). This area of study began during the **industrial revolution** $\sim (1760 - 1840)$ in order to develop the relationships among heat, work, and fuels in steam engines.[1]

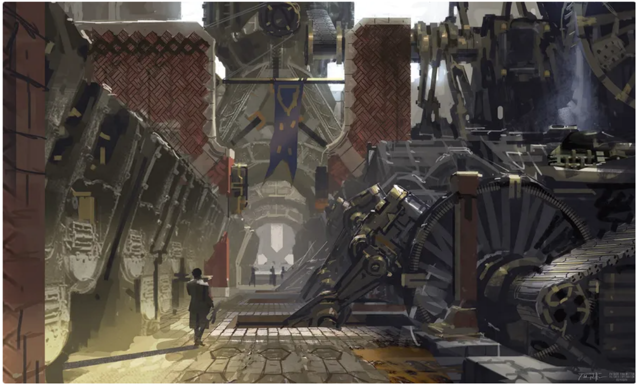
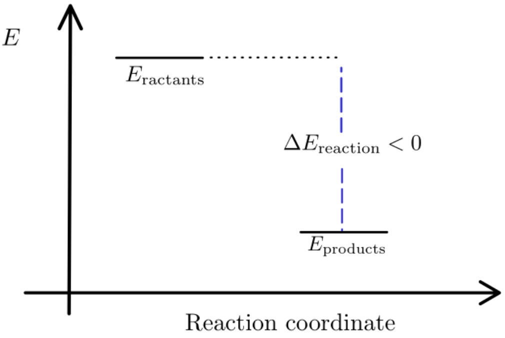


Figure: Piltover Factory[4]


E
E_{ractants}
$\Delta E_{\text{reaction}} < 0$
E_{products}
Reaction coordinate
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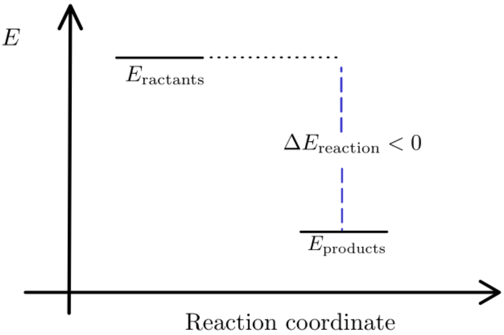
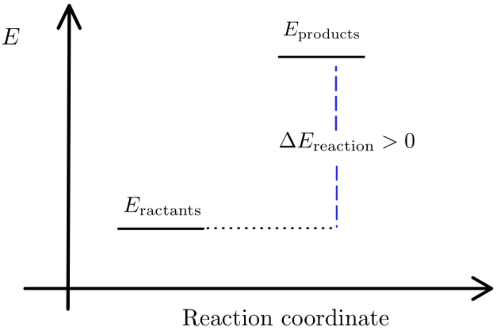


Exothermic Reaction
Energy is *released* during the reaction.



Endothermic Reaction
Energy is *absorbed* for the reaction to occur.

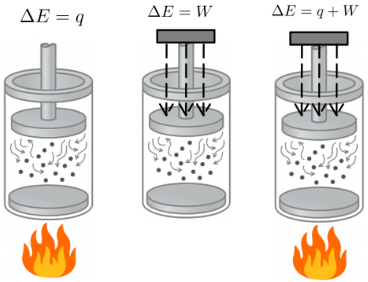
First Law of Thermodynamics

$$\Delta E = q + W$$

The change in energy (ΔE) of a system can be done through *heat* and/or *work* (W).

1. Energy is Conserved
Energy can be **transferred** (as heat or work) or **transformed** from one form to another, but it cannot be created or destroyed.

2. Systems Favor Lower Energy States
In the absence of external input, systems tend to evolve toward states of **lower internal energy**, resulting in more stable configurations.



First Law of Thermodynamics

What is Heat? Heat is energy transferred between systems due to a temperature difference.
It is a disorganized form of energy flow, unlike work

Most chemical reactions occur at constant pressure, under this conditions, the changes of a new quantity (convenient quantity) is defined: **Enthalpy**

$$H = E_{\text{int}} + W$$

So that,

$$\Delta H = q_p, \quad (q_p \text{ heat transfer at constant Pressure})$$

$$\Delta H = H_f - H_0 \approx \Delta T$$

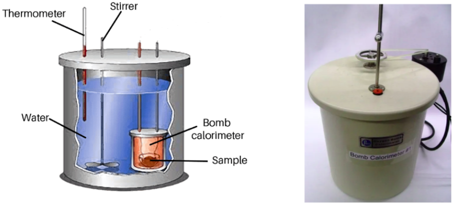


Figure: Calorimeter Bomb

Energy Units in Thermochemistry

The SI unit of energy is the **joule (J)**. Another common unit in chemistry is the **calorie (cal)**.

1 calorie is defined as the amount of energy needed to raise the temperature of **1 gram of water by 1°C (33.8 °F)**.

The conversion between these units is:

$$1\,\text{cal} = 4.184\,\text{J}$$

$$1\,\text{Kcal} = 4.184\,\text{KJ} \quad (\text{K} = \text{Kilo} = 10^3)$$

This allows us to express heat transfer (q) and enthalpy changes (ΔH) in measurable, consistent units.

Hess's Law Statement

Hess's Law: If a chemical equation can be expressed as the sum of two or more steps, **the overall enthalpy change** is the sum of the enthalpy changes for the individual steps.

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Example: Find ΔH for:

$$\mathrm{C\,(s)} + \frac{1}{2}\,\mathrm{O_2(g)} \longrightarrow \mathrm{CO\,(g)}$$

Known reactions:

$$\mathrm{C\,(s)} + \mathrm{O_2(g)} \rightarrow \mathrm{CO_2(g)} \quad \Delta H^\circ = -393.5 \text{ kJ}$$

$$\mathrm{CO\,(g)} + {}^1\!/_2\,\mathrm{O_2(g)} \rightarrow \mathrm{CO_2(g)} \quad \Delta H^\circ = -283.0 \text{ kJ}$$

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Reverse 2nd reaction:

$$\mathrm{CO_2(g) \rightarrow CO\,(g) + \frac{1}{2}\,O_2(g)} \quad \Delta H^\circ = +283.0 \text{ kJ}$$

Add reactions:

$$\begin{aligned} \mathrm{C\,(s) + O_2(g)} &\rightarrow \mathrm{CO_2(g)} \\ \mathrm{CO_2(g)} &\rightarrow \mathrm{CO\,(g) + {}^1\!/_2 O_2(g)} \end{aligned}$$

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Net: $\mathrm{C\,(s)} + \frac{1}{2}\,\mathrm{O_2(g)} \rightarrow \mathrm{CO\,(g)}$

$$\Delta H^\circ = -393.5 + 283.0 = \boxed{-110.5 \text{ kJ}}$$

$$2\,\mathrm{C\,(s) + O_2(g) \rightarrow 2\,CO\,(g)}$$

$$\Delta H^\circ = \boxed{-221.0 \text{ kJ}}$$

Try:

Calculate ΔH for the reaction:

$$2\,\mathrm{C}\,(\mathrm{s}) + \mathrm{H_2(g)} \rightarrow \mathrm{C_2H_2(g)}$$

Given Data:

$$\mathrm{C_2H_2(g)} + \frac{5}{2}\,\mathrm{O_2(g)} \rightarrow 2\,\mathrm{CO_2(g)} + \mathrm{H_2O\,(l)}$$

$\Delta H = -1299.6$ kJ

$$\mathrm{C\,(s)} + \mathrm{O_2(g)} \rightarrow \mathrm{CO_2(g)}$$

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$$\mathrm{H_2(g)} + \frac{1}{2}\,\mathrm{O_2(g)} \rightarrow \mathrm{H_2O\,(l)}$$

$\Delta H = -285.8$ kJ

Try:

Calculate ΔH for the reaction:

$$\mathrm{S\,(s)} + \frac{3}{2}\,\mathrm{O_2(g)} \longrightarrow \mathrm{SO_3(g)}$$

Given Data:

$$\begin{aligned} \mathrm{S\,(s)} + \mathrm{O_2(g)} &\rightarrow \mathrm{SO_2(g)} \quad \Delta H = -296.8 \text{ kJ} \\ 2\,\mathrm{SO_2(g)} + \mathrm{O_2(g)} &\rightarrow 2\,\mathrm{SO_3(g)} \quad \Delta H = -197.0 \text{ kJ} \end{aligned}$$

We are given the target reaction:

$$2\,C\,(s) + H_2(g) \longrightarrow C_2H_2(g)$$

$$2\,CO_2(g) + H_2O\,(l) \rightarrow C_2H_2(g) + \frac{5}{2}\,O_2(g) \quad \Delta H = +1299.6 \text{ kJ}$$

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$$2\,C\,(s) + 2\,O_2(g) \rightarrow 2\,CO_2(g) \quad \Delta H = -787.0 \text{ kJ}$$

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Add reactions and cancel opposite species:

Net reaction:

$$2\,\mathrm{C}\,(\mathrm{s}) + \mathrm{H_2(g)} \longrightarrow \mathrm{C_2H_2(g)}$$

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Net reaction:

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Final enthalpy change:

$$\Delta H = +1299.6 - 787.0 - 285.8 = \boxed{226.8 \text{ kJ}}$$

We are given the target reaction:

$$S(s) + \frac{3}{2}O_2(g) \longrightarrow SO_3(g)$$

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Manipulate the second equation: Divide by 2 to match 1 mol of $SO_3(g)$

$$SO_2(g) + \frac{1}{2}\,O_2(g) \longrightarrow SO_3(g) \quad \Delta H^\circ = -98.5 \text{ kJ}$$

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Add reactions and cancel intermediate species:

Net reaction:

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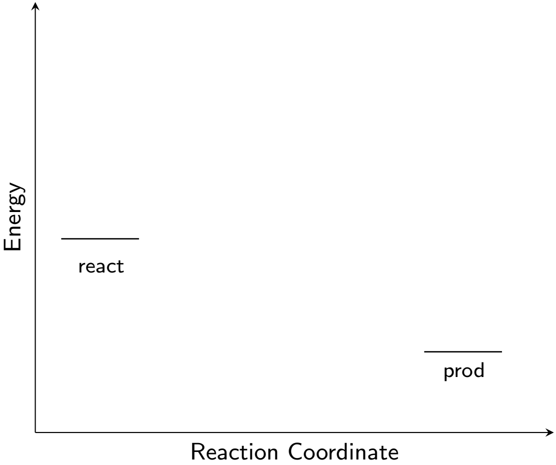
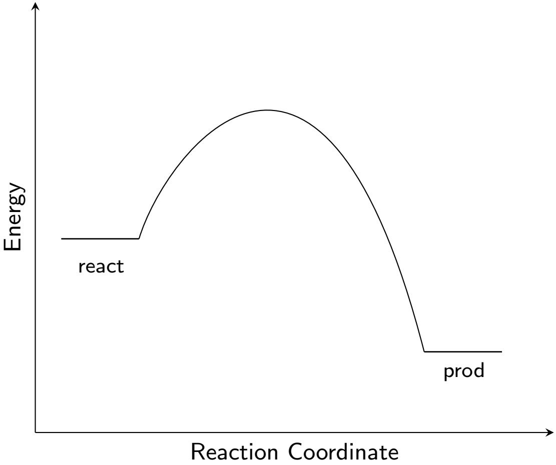
Final enthalpy change:

$$\Delta H = -296.8 + (-98.5) = \boxed{-395.3 \text{ kJ}}$$

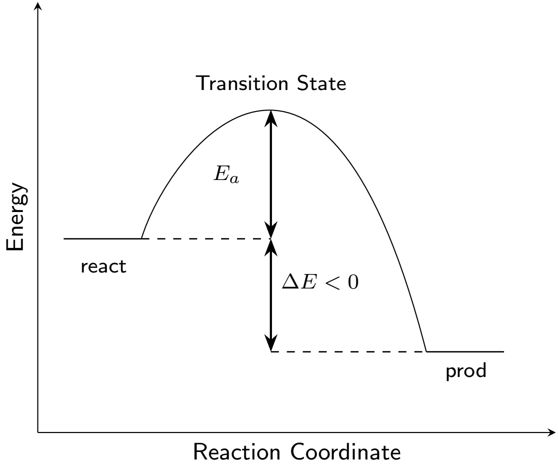


$$2\,\mathrm{NO}\,(\mathrm{g}) \rightarrow \mathrm{N_2(g)} + \mathrm{O_2(g)} \;\; \Delta H = -180 \text{ kJ/mol}$$



$$2\,\mathrm{NO}\,(\mathrm{g}) \rightarrow \mathrm{N_2(g)} + \mathrm{O_2(g)}\;\; \Delta H = -180\ \text{kJ/mol}$$

$$E_a = 300\text{kJ/mol}$$



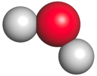


Figure: Water

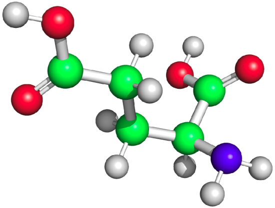


Figure: Glutamic Acid

$$2\,\mathrm{NO}\,(\mathrm{g}) \rightarrow \mathrm{N}_2(\mathrm{g}) + \mathrm{O}_2(\mathrm{g}) \;\; \Delta H = -180 \text{ kJ/mol}$$

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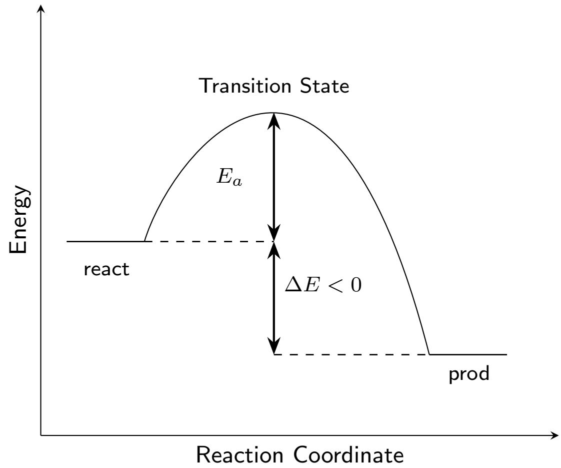

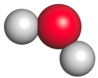

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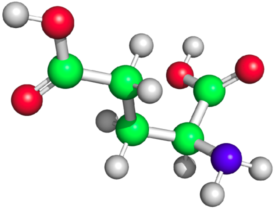

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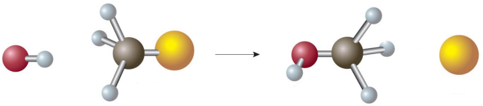

Figure: Displacement Reaction

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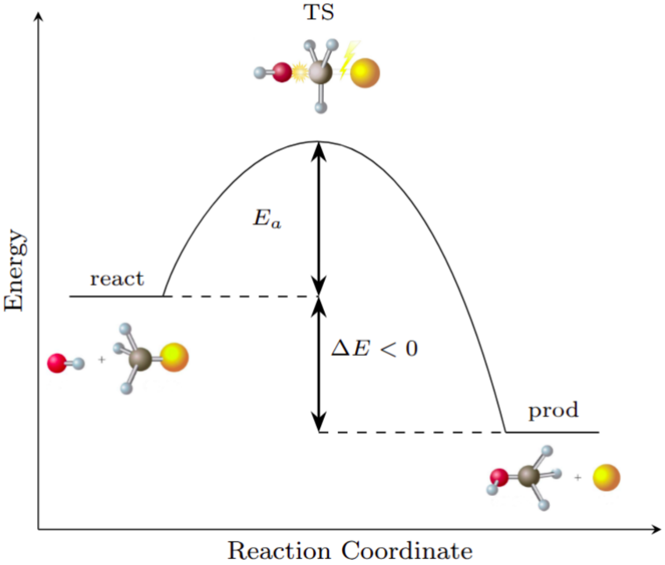

Figure: One step reaction

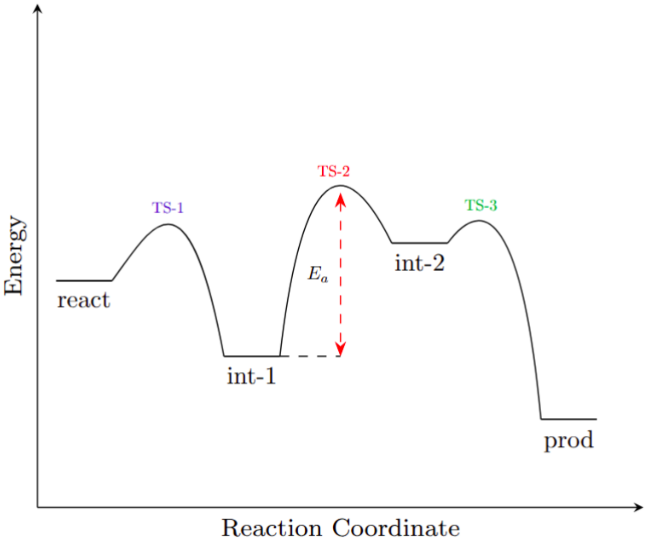

Figure: Multi-step reaction

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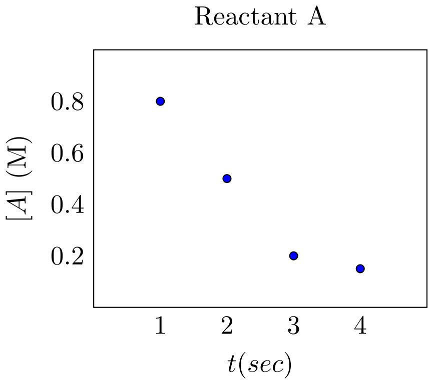
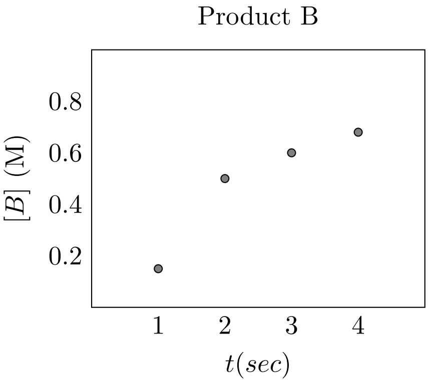
aA→bB





Consider the chemical reaction aA $\longrightarrow$ bB:

$$\text{(AVG) rate}_A = -\frac{\Delta A}{\Delta t} \qquad \text{(AVG) rate}_B = \frac{\Delta B}{\Delta t}$$

$$V_A = -\frac{dA}{dt} \qquad V_B = \frac{dB}{dt}$$

Reaction Rate: rate $= V_R$

$$V_R = -\frac{1}{a}\frac{dA}{dt} = \frac{1}{b}\frac{dB}{dt}$$

Try: aA + bB$\rightarrow$ cC + dD (General Chemical Reaction)[4]

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(a) How is the rate at which ozone disappears related to the rate at which oxygen appears in the reaction:

$$2\,O_3(g) \longrightarrow 3\,O_2(g)$$

(b) If the rate at which O_2 appears,

$$\frac{\Delta[O_2]}{\Delta t} = 6.0 \times 10^{-5}\ \text{M/s}$$

at a particular instant, what is the rate of consumption of O_3 at this same time?

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Sol:

(a) $$V_R = -\frac{1}{2}\frac{dO_3}{dt} = \frac{1}{3}\frac{dO_2}{dt}$$

(b) $$-\frac{dO_3}{dt} = \frac{2}{3}\frac{dO_2}{dt} = 4.0 \times 10^{-5}\text{M/s}$$

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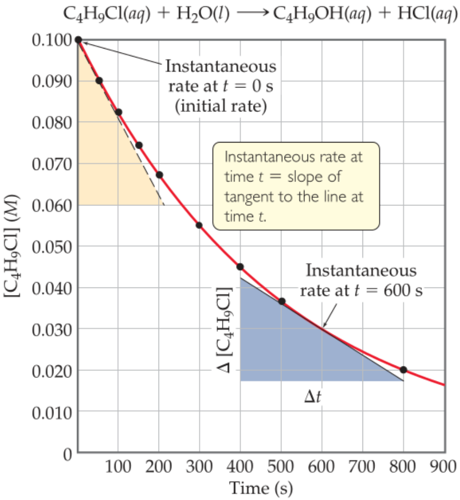
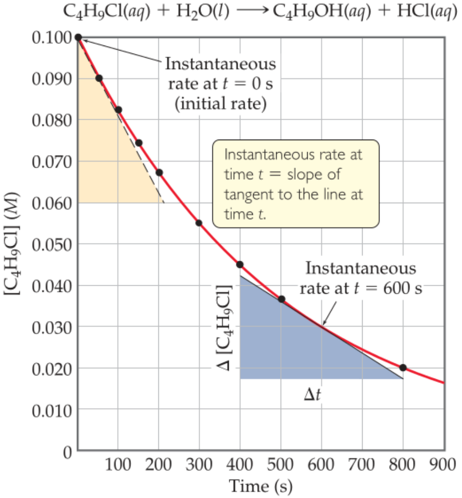


Figure: Concentration of butyl chloride C_4H_9Cl as a function of time.[4]

What factors affect the reaction rate (V_R)?



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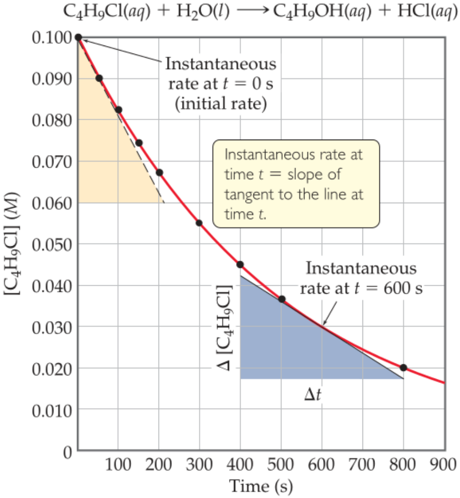

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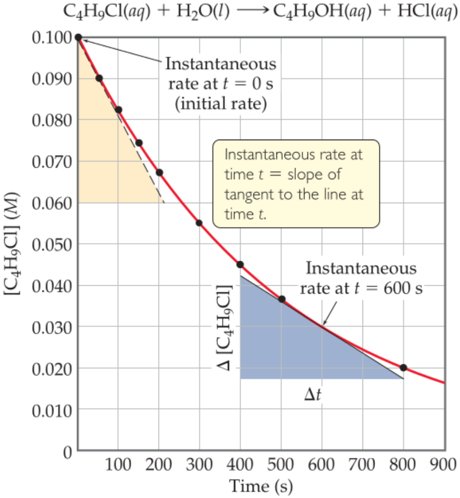
$$NH_4{}^+\,(aq) + NO_2{}^-\,(aq) \longrightarrow N_2(g) + 2\,H_2O\,(l)$$

Exp	$NH_4{}^+$ (M)	$NO_2{}^-$ (M)	Observed Initial Rate (M/s)
1	0.0100	0.2000	5.40×10^{-7}
2	0.0200	0.2000	10.8×10^{-7}
3	0.0400	0.2000	21.5×10^{-7}
4	0.2000	0.0202	10.8×10^{-7}
5	0.2000	0.0404	21.6×10^{-7}
6	0.2000	0.0808	43.3×10^{-7}

Table: Rate data for the reaction of ammonium and nitrite ions in water at 25 °C.



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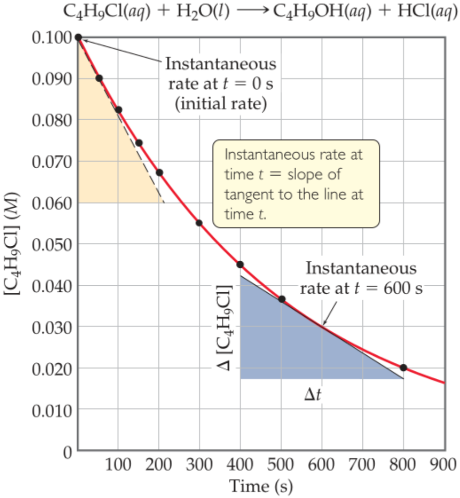

Figure: Concentration of butyl chloride C_4H_9Cl as a function of time.[4]

What factors affect the reaction rate (V_R)?

- Concentration:

$$NH_4{}^+\,(aq) + NO_2{}^-\,(aq) \longrightarrow N_2(g) + 2\,H_2O\,(l)$$

Exp	$NH_4{}^+$ (M)	$NO_2{}^-$ (M)	Observed Initial Rate (M/s)
1	0.0100	0.2000	5.40×10^{-7}
2	0.0200	0.2000	10.8×10^{-7}
3	0.0400	0.2000	21.5×10^{-7}
4	0.2000	0.0202	10.8×10^{-7}
5	0.2000	0.0404	21.6×10^{-7}
6	0.2000	0.0808	43.3×10^{-7}

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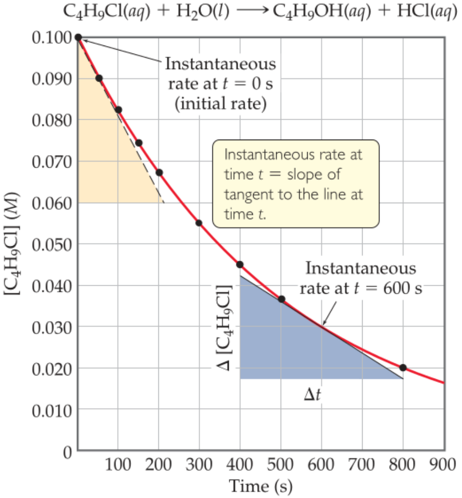

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$V_R = k[NH_4{}^+][NO_2{}^-]$ (Reaction Rate law with reaction constant k)

General Rate Law:

$$V_R = k[\text{reactant 1}]^m[\text{reactant 2}]^n \cdots$$

- k: rate constant
- i: reaction orders with respect to reactants, $i = \{m, n, \dots\}$(determined experimentally)
- Sum of exponents $\Rightarrow$ **overall reaction order**

In the previous example: $V_R = k[\mathrm{NH_4}^+][\mathrm{NO_2}^-]$

– Reaction order respect to NH_4^+: $m = 1$

– Reaction order respect to NO_2^-: $n = 1$

– Overall reaction order: $m + n = 2$

Consider the reaction: aA$\rightarrow$ products

$$V_R = k[A] \text{ (Overall 1st Order)}$$

$$V_R = k[A]^2 \text{ (Overall 2nd Order)}$$

$$V_R = k \text{ (Overall zeroth Order)}$$

For aA + bB$\rightarrow$ products we can have

$$V_R = k[A][B], \text{ Overall 2nd Order}$$

Now, we have that $V_R = -\frac{1}{a}\frac{dA}{dt}$ so we have three cases to determine $[A](t)$.

First Order Reaction: aA $\longrightarrow$ products

$$V_R = -\frac{1}{a}\frac{dA}{dt}$$

$$V_R = k[A]$$

$$\frac{d[A]}{dt} = -k_a[A], \text{ (separable differential equation)} \qquad (1)$$

where $k_a = \dfrac{1}{a}k$. Solving (1) we have $\dfrac{d[A]}{[A]} = -k_a dt$

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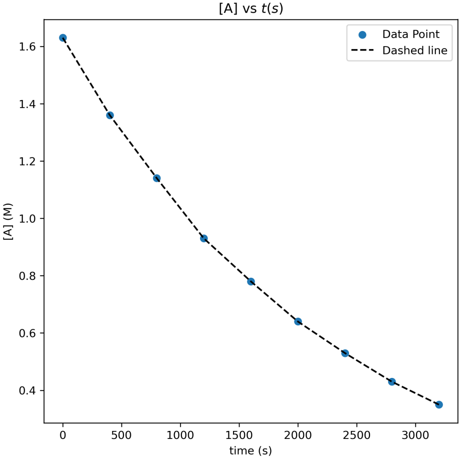

Figure: Evolution of [A] over time

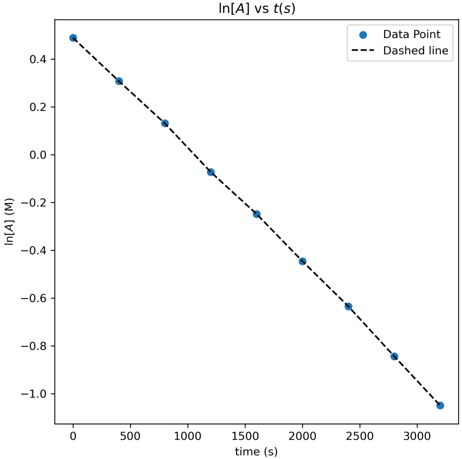

Figure: Evolution of $\ln([A])$ over time

Second Order Reaction: aA $\longrightarrow$ products

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$$V_R = k[A]^2$$

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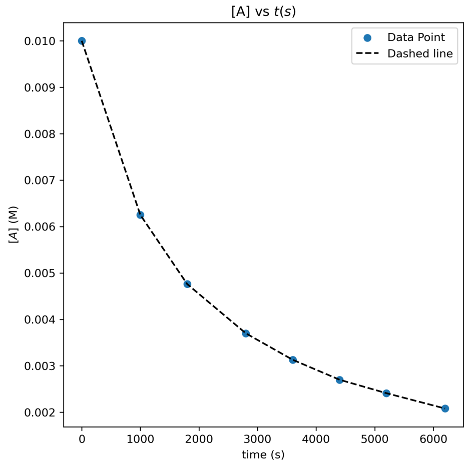

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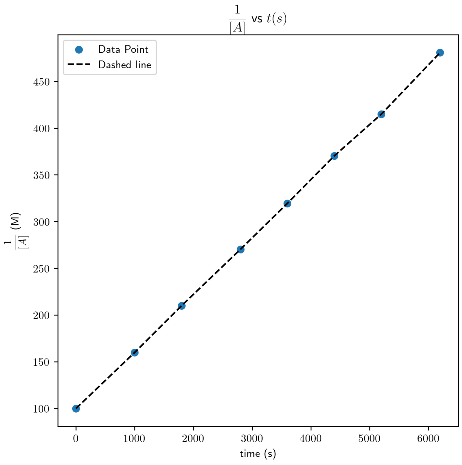

Figure: Evolution of $\frac{1}{[A]}$ over time

Zero Order Reaction: aA $\longrightarrow$ products

$$V_R = -\frac{1}{a}\frac{dA}{dt}$$

$$V_R = k$$

$$\frac{d[A]}{dt} = -k, \text{ (separable differential equation)} \qquad (3)$$

where $k_a = \dfrac{1}{a}k$. Solving (2) we have $d[A] = -k_a dt$

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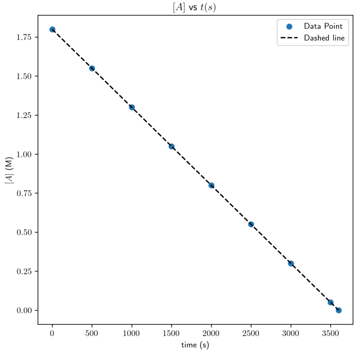

Figure: [A] evolution over time

Reaction Mechanism: The steps by which a reaction occurs is called the *reaction mechanism*.

- Elementary Reaction: Is a reaction that occurs in a single step, with no experimentally detectable reaction intermediates.

  The **molecularity** is defined as the number of species that must collide to produce the reaction indicated by the elementary reaction.

- Multi-step Reaction: A reaction that occurs in more that one step.
  (A multi-step reaction can be described as a set of elementary reactions)

[5] Steven S. Zumdahl, Susan A. Zumdahl, and Donald J. DeCoste. *Chemistry*. 10. th. 2018, p. 490

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$$NO_2(g) + CO(g) \longrightarrow NO(g) + CO_2(g)$$

with experimentally determined rate $V_R = k[NO]^2$. This is not a elementary reaction.

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$$\mathrm{NO_2(g) + NO(g) \xrightarrow{k_1} NO_3(g) + NO(g)}$$

$$\mathrm{NO_3(g) + CO(g) \xrightarrow{k_2} NO_2(g) + CO_2(g)}$$

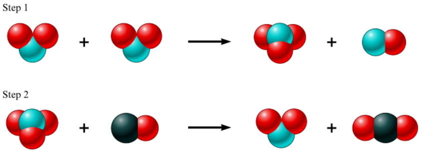


Figure: Mechanism of the reaction of NO_2 and CO[5]

[5] Steven S. Zumdahl, Susan A. Zumdahl, and Donald J. DeCoste. *Chemistry*. 10. th. 2018, p. 490

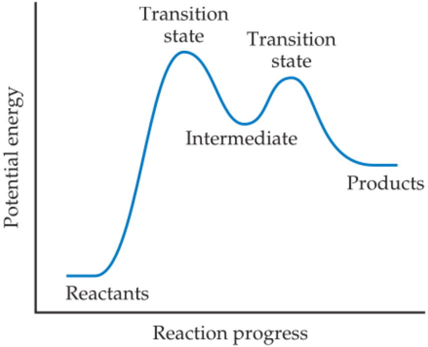


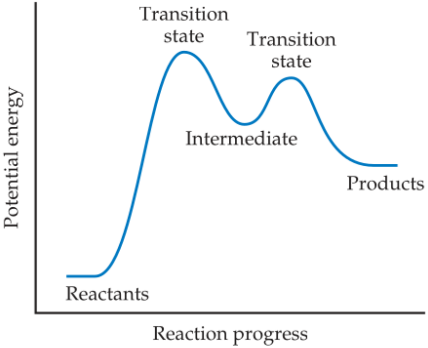
Figure: Energy profile of $NO_2(g) + CO(g)$[4]

In the reaction $NO_2(g) + CO(g)$ the rate determining step is the collision of two $NO_2(g)$ molecules. This is reflected in the reaction rate

$$V_R = k[\mathrm{NO}]^2$$

Two reaction steps can be identified:

- Slow: Rate determining step
- Fast



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Three possible "collisions" are usually considered in the rate determining step:

- Unimolecular (one molecule)
- Bimolecular (two molecules)
- Termolecular (three molecules) rare events

Arrhenius Equation: Dependence of reaction rate V_R and the the $\boxed{k = Ae^{-E_a/RT}}$ rate constant

A: Pre-exponential factor (Collision Frequency), ${}^{E_a}/_{RT}$: Activation Energy, and Temperature

[5] Jing wen Feng, Yue jie Liu, and Jing xiang Zhao. "Layered SiC sheets: A promising metal-free catalyst for NO reduction". In: *Journal of Molecular Graphics and Modelling* 60 (2015), pp. 132–141

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Activation Energy E_a: Catalysis

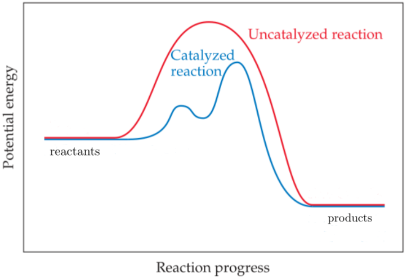

Figure: Lowering of Activation Energy

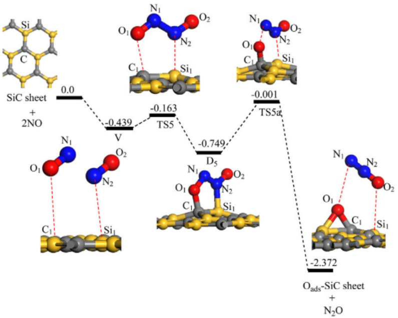

Figure: NO reduction over Layered SiC sheets[6]

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Rate Constant and Temperature dependence:

$$k = Ae^{-E_a/RT} \Rightarrow \ln(k) = \ln(A) - \left(\frac{E_a}{R}\right)\frac{1}{T}$$

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$$k = Ae^{-E_a/RT} \Rightarrow \ln(k) = \ln(A) - \left(\frac{E_a}{R}\right)\frac{1}{T}$$

Consider the following data of the rate constant:

Temperature (K)	k ($M^{-1}s^{-1}$)
600	0.028
650	0.22
700	1.3
750	6.0
800	23

Table: Temperature dependence of the rate constant.

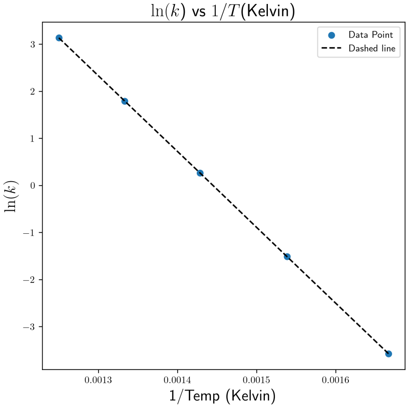

Figure: $\ln(k)$ plot and linear dependence on $1/T$

- Using matplotlib and numpy for visualization
- Linear regression with scipy
- Extracting rate constants and activation energy

- First-order kinetics of N_2O_5
- Second-order kinetics of NO (If times allows)
- Arrhenius plots and activation energy (If times allows)