TRƯỜNG ĐẠI HỌC NÔNG LÂM TPHCM
BỘ MÔN CÔNG NGHỆ HÓA HỌC

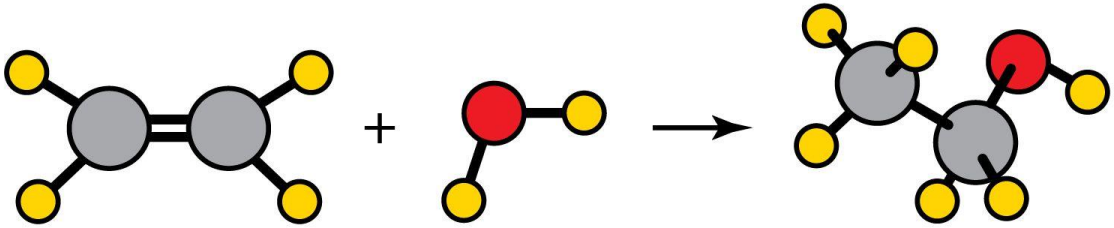
GIỚI THIỆU CNHH

CHƯƠNG 2:
NGUYÊN TẮC CƠ BẢN CỦA CÔNG NGHỆ HÓA HỌC
(Phần 1)

Chemical Reaction

A process in which one or more substances, the reactants, are converted to one or more different substances, the products.

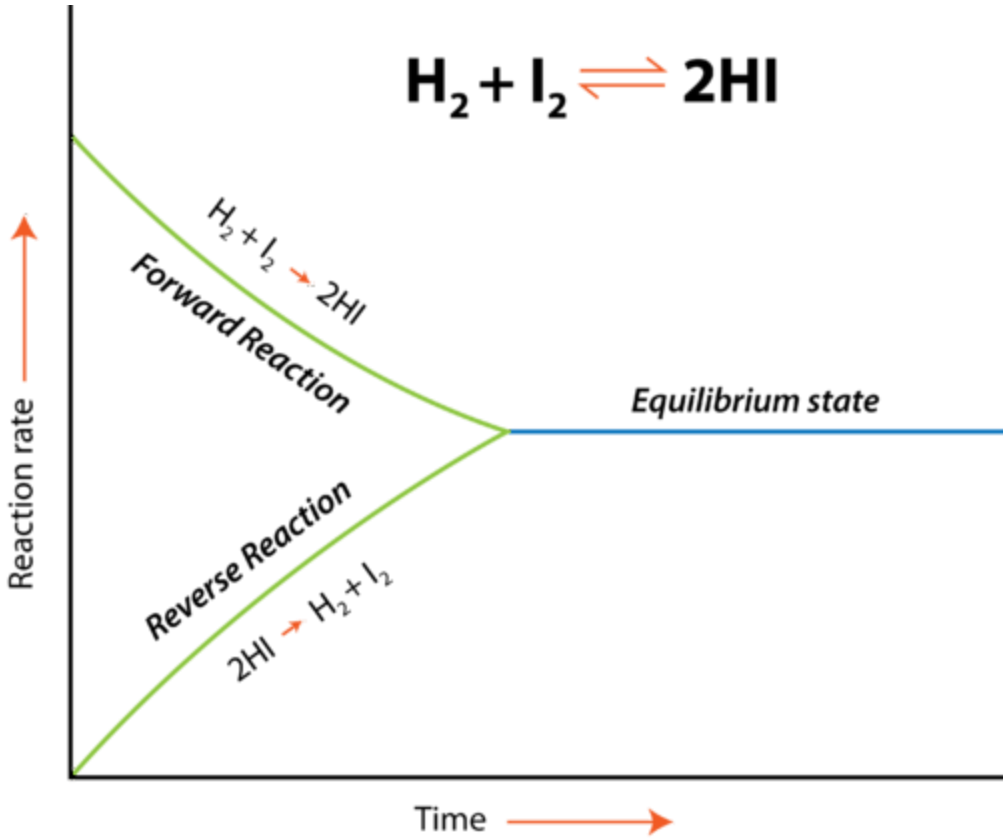
Production of ethanol (CH_3CH_2OH)



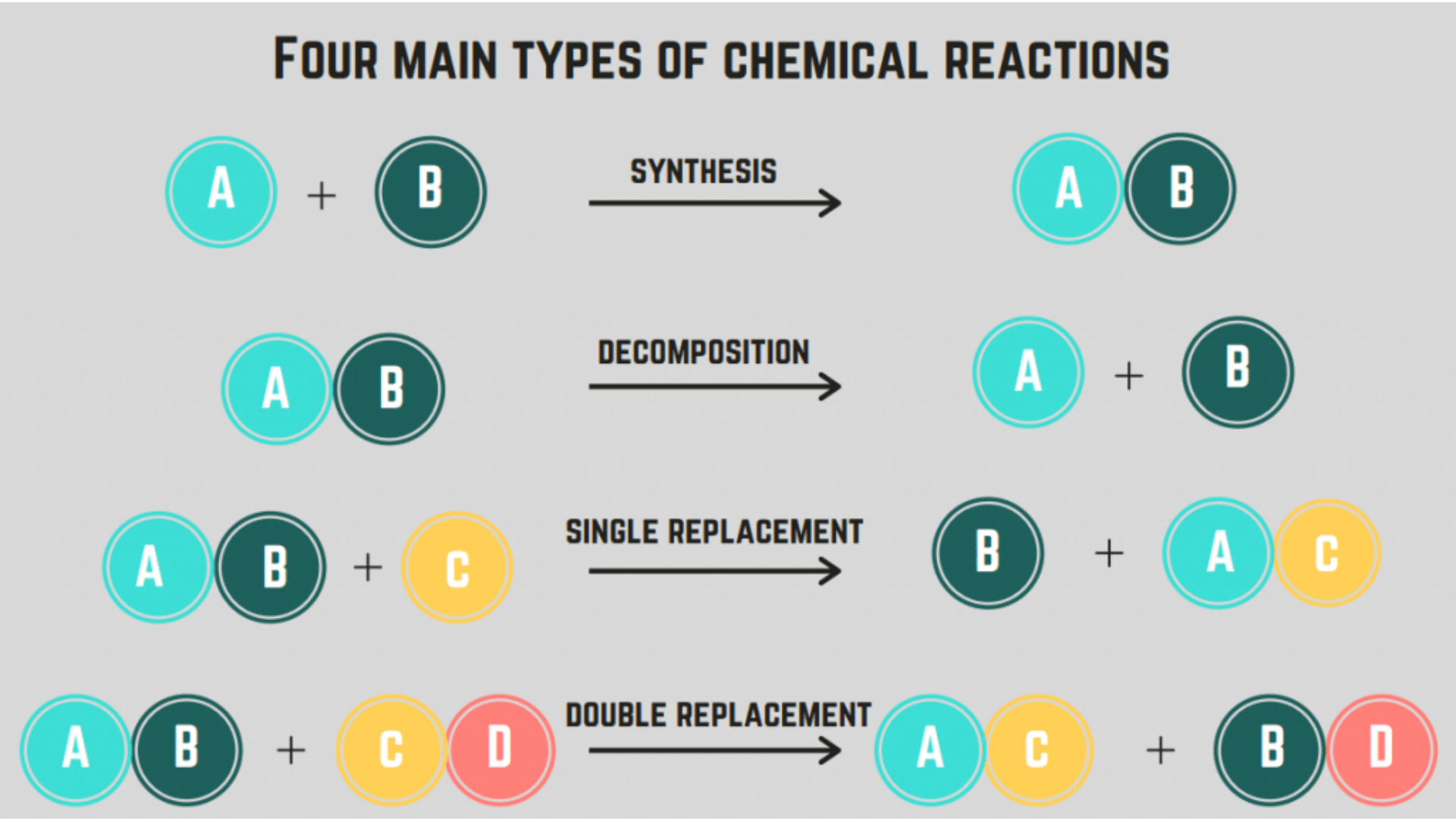
C_2H_4 + H_2O → CH_3CH_2OH

ethylene + water → ethanol

A forward reaction is a reaction in which products are produced from reactants and it goes from left to right in a reversible reaction. A backward reaction is a reaction in which reactants are produced from products and it goes from right to left in a reversible reaction.



Types of Chemical Reactions



SYNTHESIS

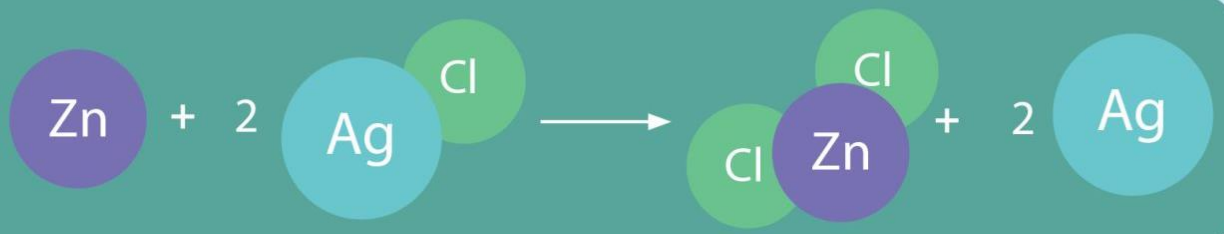
Multiple reactants, which can be simple elements or compounds, combine together to form a single compound.

DECOMPOSITION

A compound breaks down into two or more simpler substances. Decomposition reactions are classified into thermal, electrolytic, and photo.

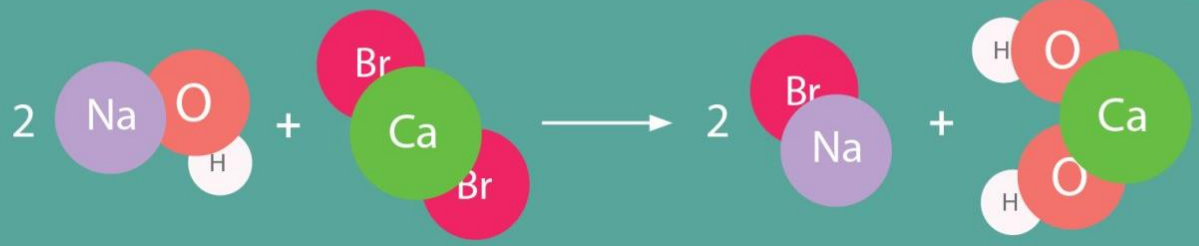
SINGLE-REPLACEMENT

One element is substituted for another element in a compound, generating a new compound and a pure element.



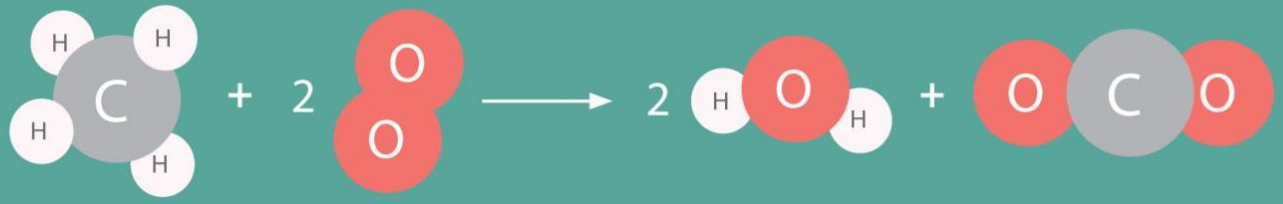
DOUBLE-REPLACEMENT

Two ionic compounds exchange cations or anions to form two new compounds. Forming a precipitate can help drive the reaction to the right.



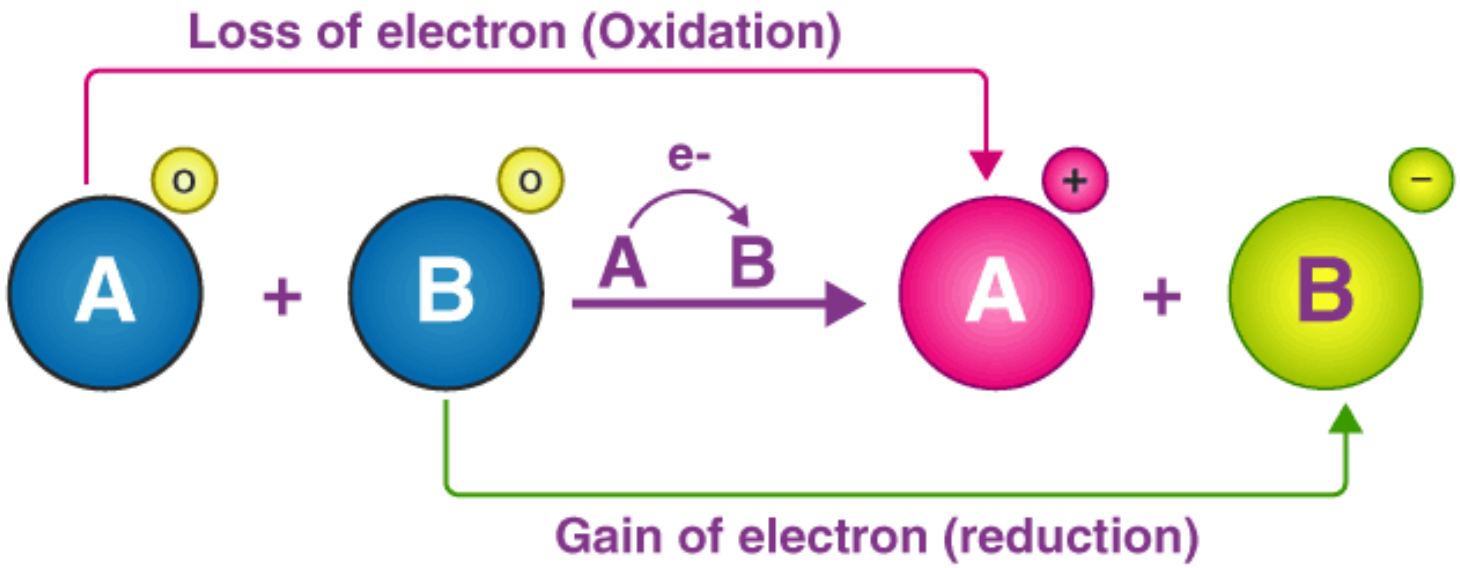
COMBUSTION

A fuel, typically a hydrocarbon, reacts with oxygen gas to form carbon dioxide and water, which generates heat and light.



NEUTRALIZATION

Acid and base combine to neutralize each other in aqeuous solutions, usually resulting in a salt and water.



Oxidation & Reduction

Oxidized

Reducing Agent

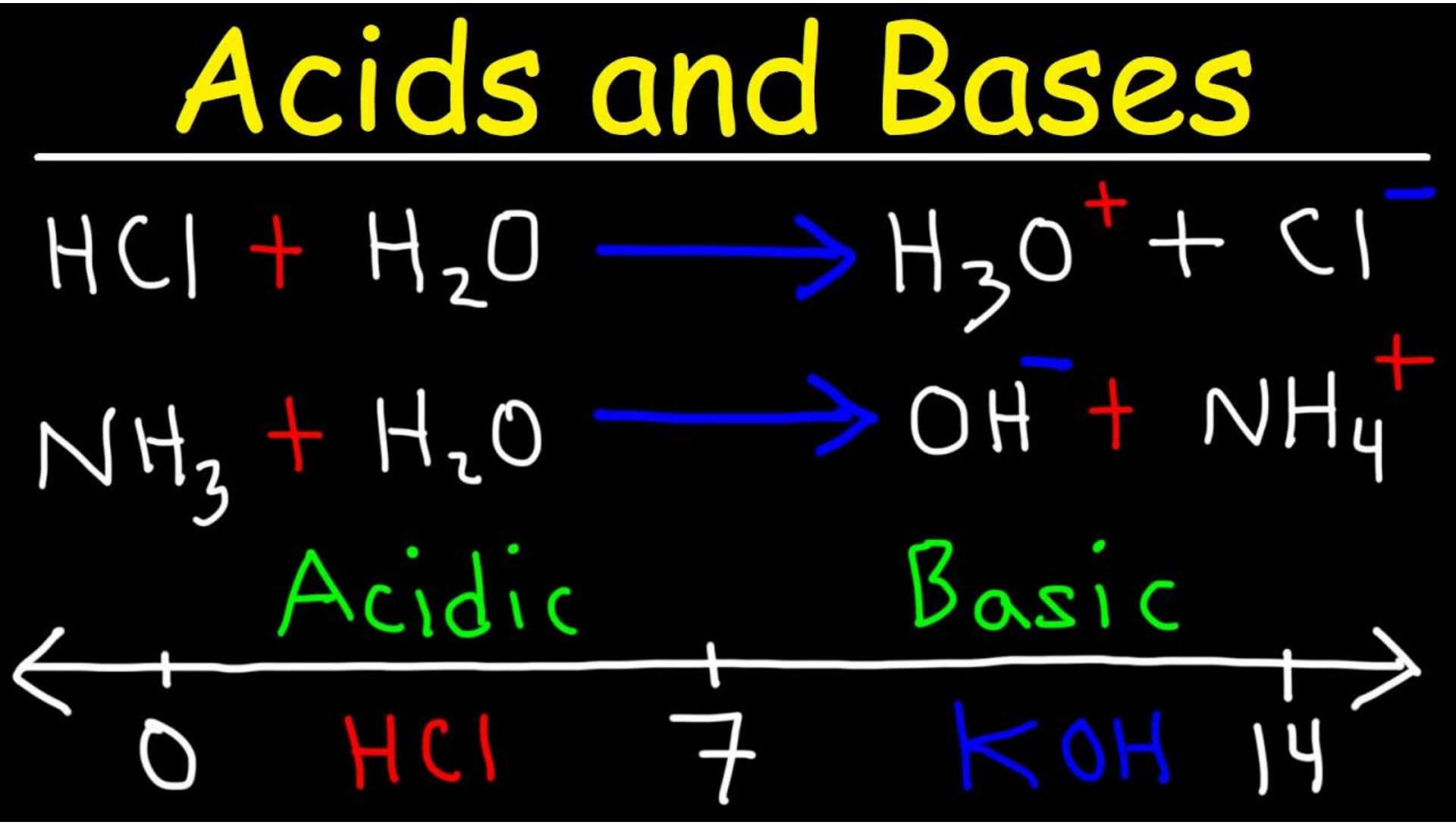
Loss of e^-

Reduced

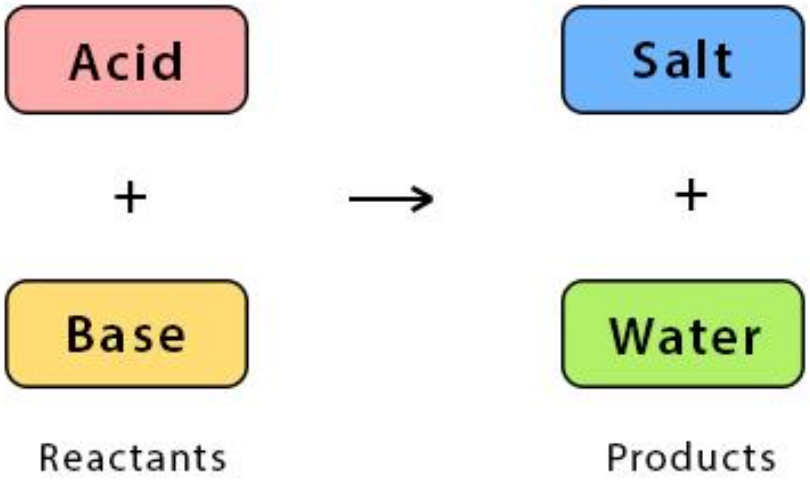
Oxidizing Agent

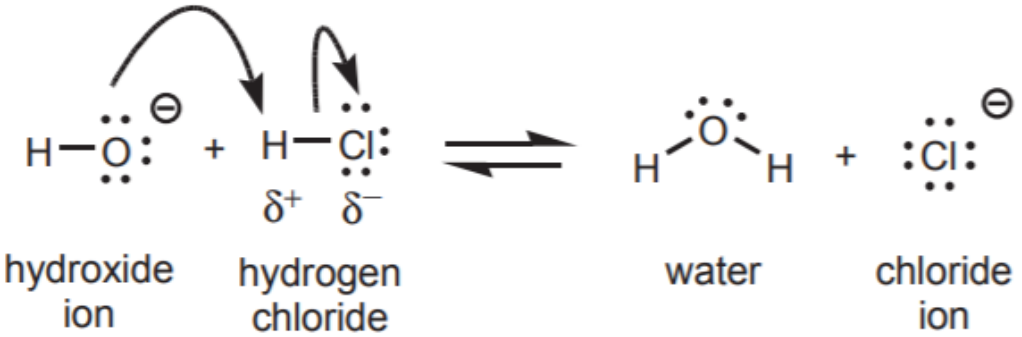
Gain of e^-

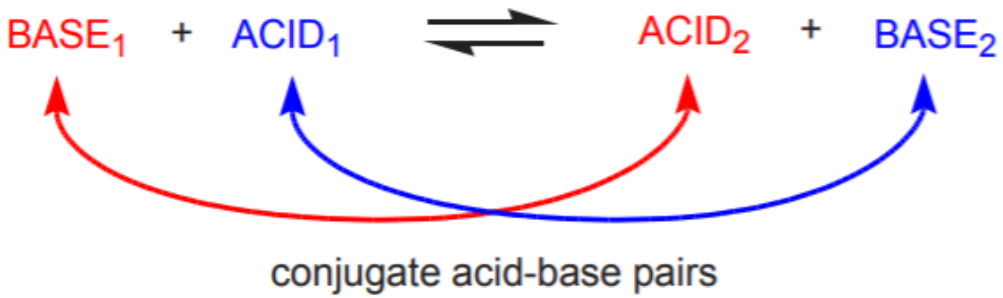
Acids and Bases



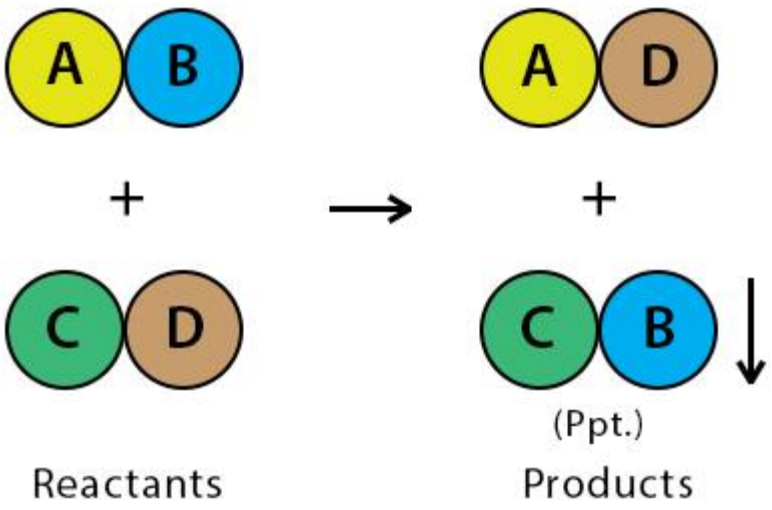
Acid-Base Reaction

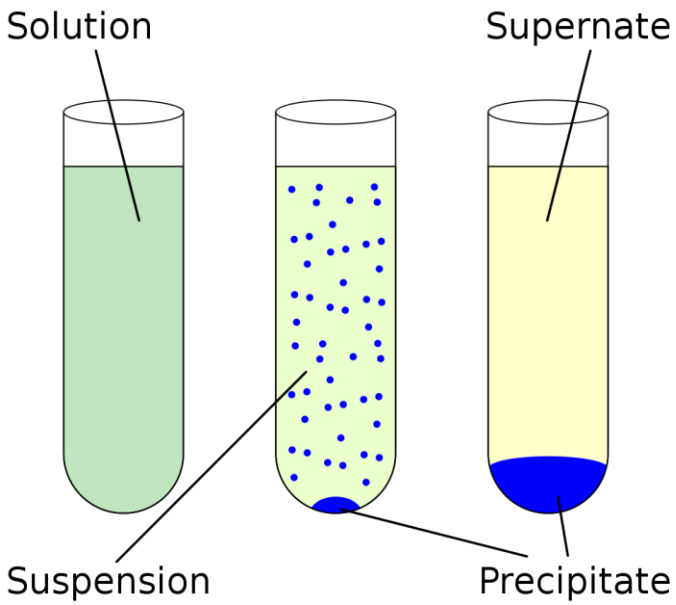






Precipitation Reaction





PRECIPITATION RXNS

Precipitate

SOL'N$_{(aq)}$ + SOL'N$_{(aq)}$ → SOLID$_{(s)}$

SOLUBLE INSOLUBLE

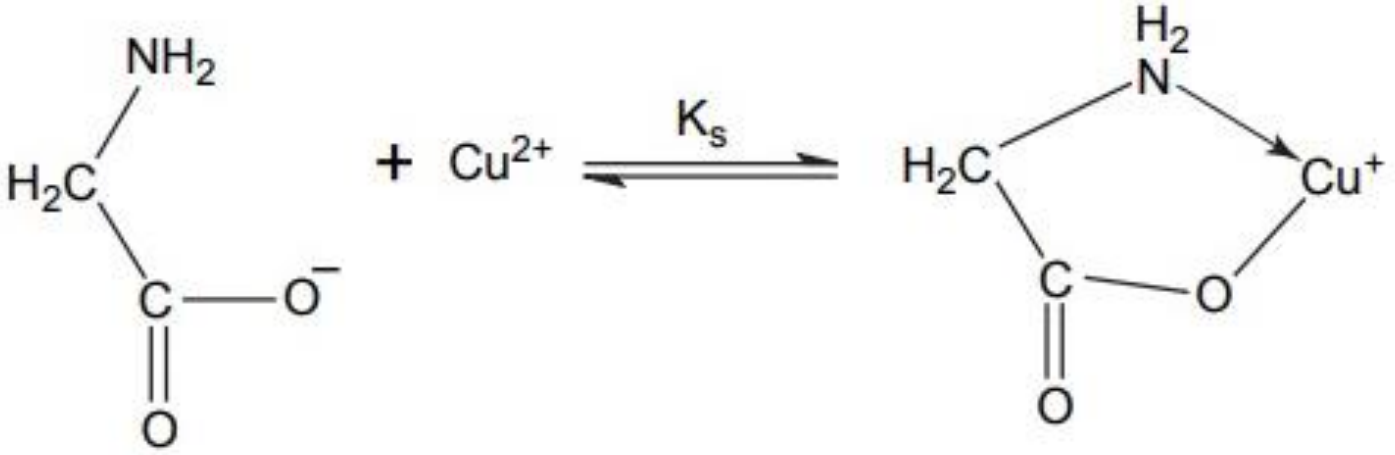
Complexation Reaction

$$Ag^{+} + 2\,NH_3 \longrightarrow [Ag(NH_3)_2]^{+}$$

Silver ion — Ammonia

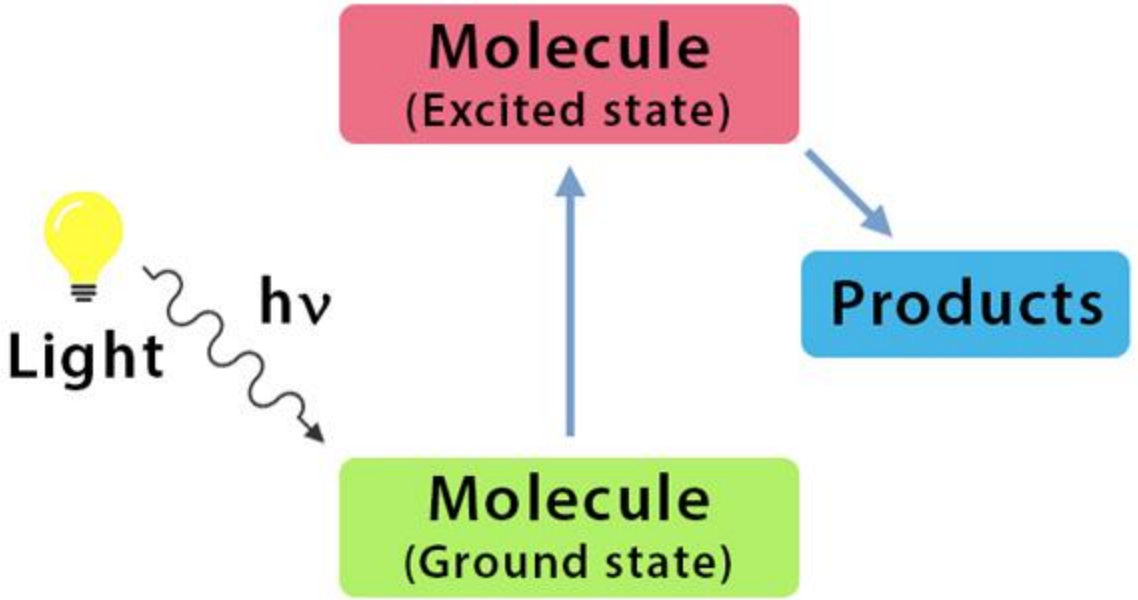
$$Ni^{2+} + 4\,CN^{-} \longrightarrow [NiCN_4]^{2-}$$

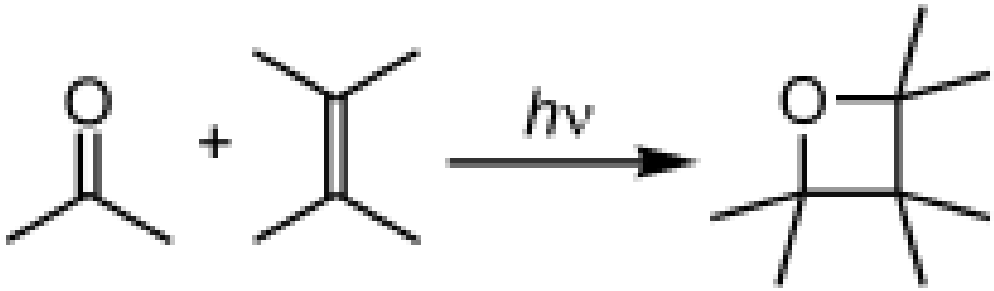
Nickle ion — Cyanide ion



Glycine anion — Copper — Glycine–copper complex

Photochemical Reaction





In this Paterno–Büchi reaction, a photoexcited carbonyl group is added to an unexcited olefin, yielding an oxetane

Photochemical Reaction Examples

$$6\,CO_2 + 6\,H_2O + h\nu \longrightarrow C_6H_{12}O_6 + 6\,O_2$$

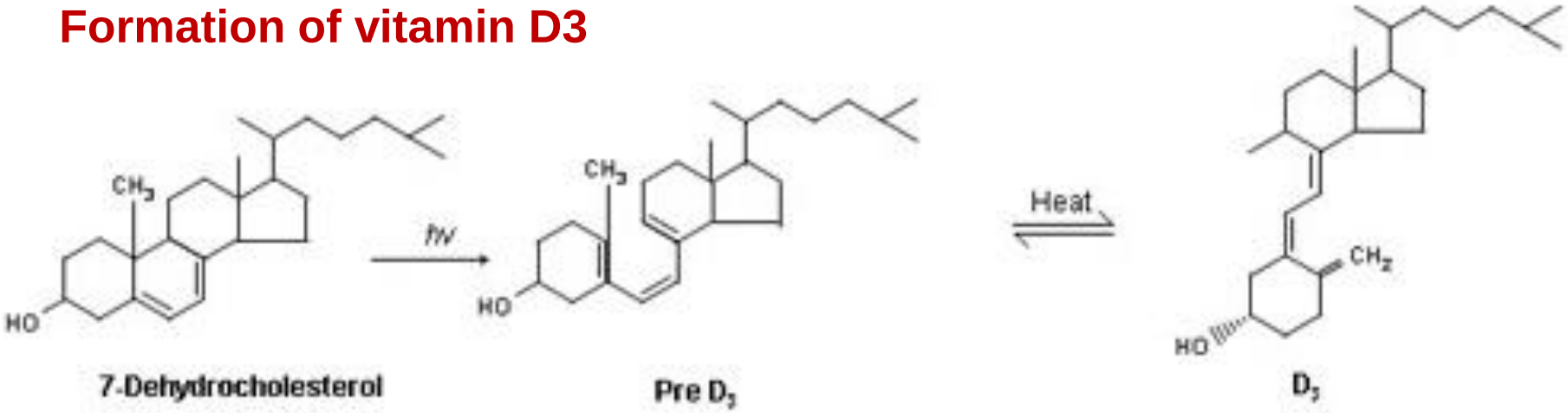
Carbon dioxide | Water | Light energy | Glucose | Oxygen

< Photosynthesis >

$$2\,AgCl + h\nu \longrightarrow 2\,Ag + Cl_2$$

Silver chloride | Silver | Chlorine

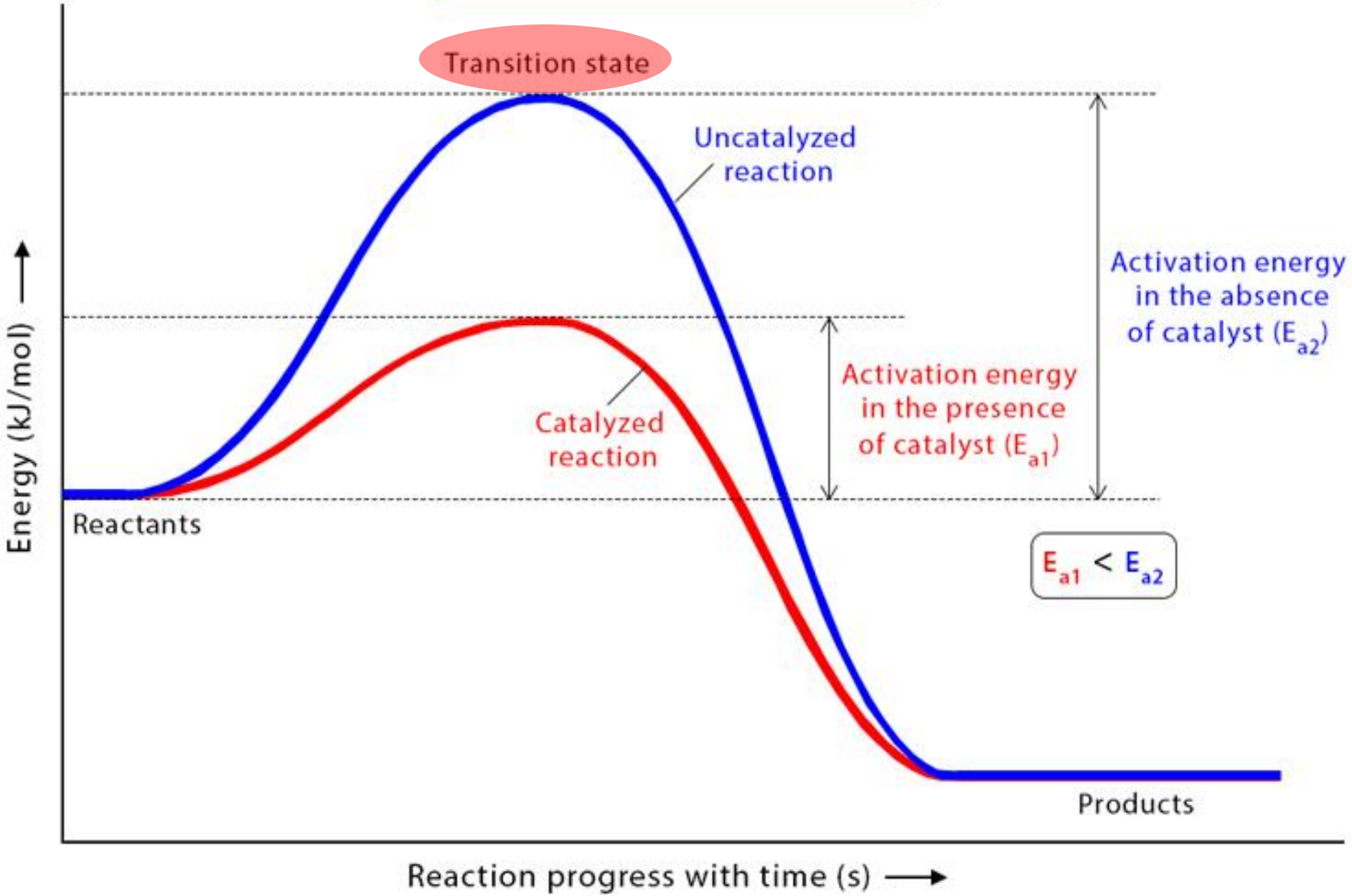
Formation of vitamin D3

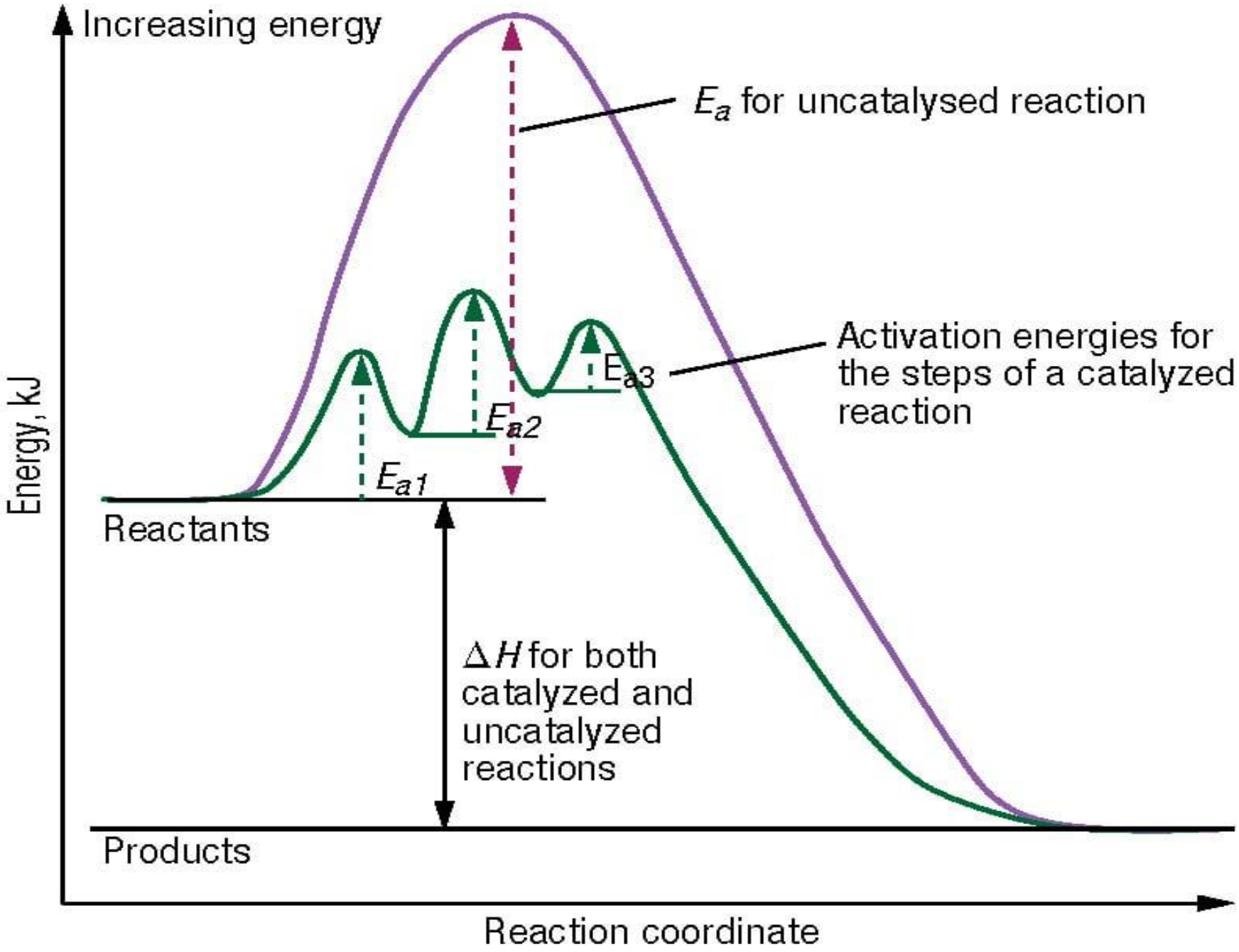


7-Dehydrocholesterol | Pre D_3 | D_3

< Cholecalciferol >

Catalytic Reaction




Increasing energy
E_a for uncatalysed reaction
Activation energies for the steps of a catalyzed reaction
E_{a3}
E_{a2}
E_{a1}
Energy, kJ
Reactants
ΔH for both catalyzed and uncatalyzed reactions
Products
Reaction coordinate

Chemical Kinetics

(Reaction kinetics) is concerned with the rates of chemical reactions, the quantitative description of how fast chemical reactions occur, and the factors affecting these rates.

- Investigate reaction's mechanism pathways and transition states
- Construct mathematical models describing the characteristics of a chemical reaction or reactor
- Devise new/better ways of achieving desired chemical reactions; improve the yield of desired products or develop a better catalyst

Rate of Reaction

The speed of a chemical reaction, is proportional to the increase in the concentration of a product per unit time and to the decrease in the concentration of a reactant per unit time

- The rate of reaction is defined for a reactant or a product
- The rate of reaction with respect to a species A is defined negative if A is consumed, and is positive if A is produced
- The rate of reaction with respect to a species A may be extensive rate (R_A) or intensive rate (r_A), which is the rate referred to a specified normalizing quantity (NQ) or rate basis

- The extensive rate of reaction (R_A): the observed rate of formation of A

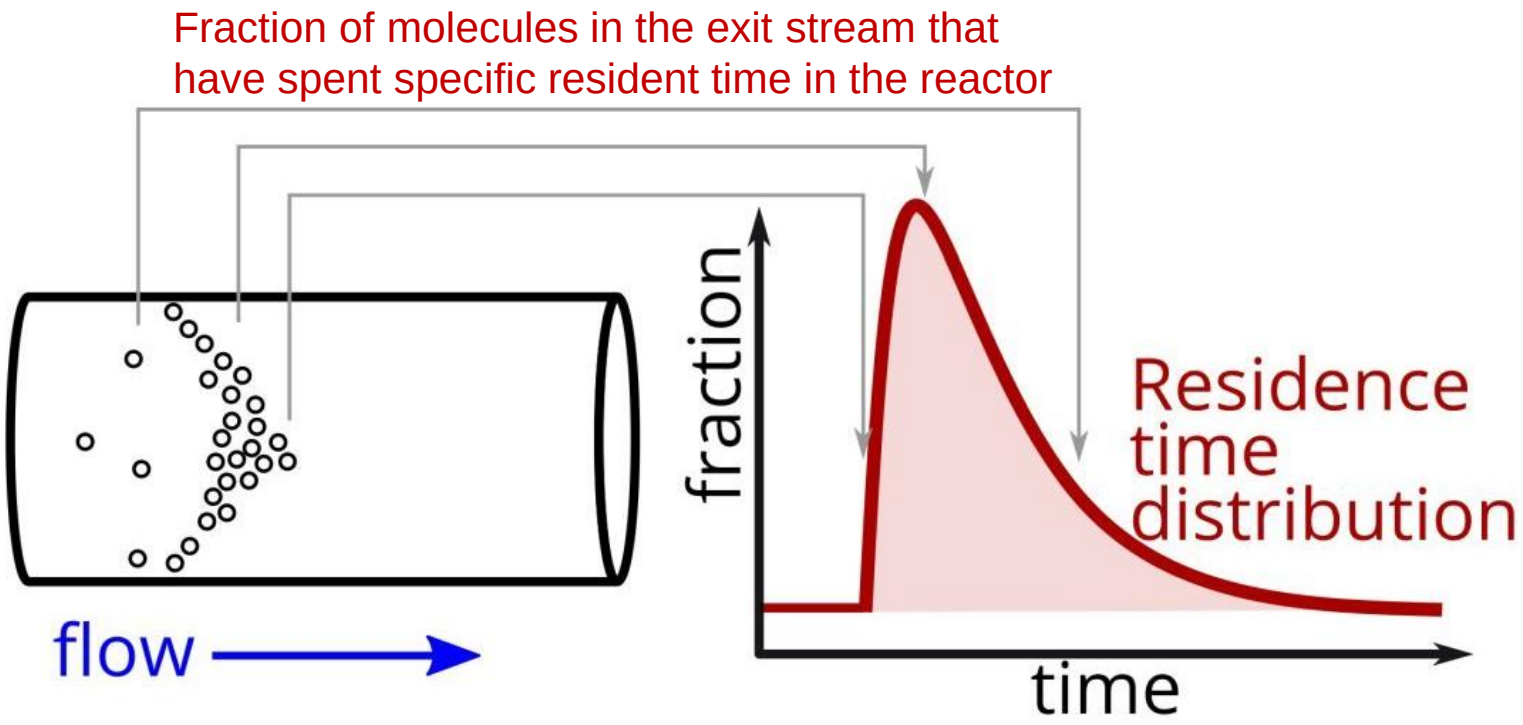
$$R_A = \frac{moles\ \ A\ \ formed}{unit\ \ time}, \ e.g., \ \frac{\text{mol}}{\text{s}}$$

- The intensive rate of reaction (r_A): the rate referred to a specified normalizing quantity (NQ) or rate basis, such as volume of reacting system or mass of catalyst

$$r_A = \frac{moles\ \ A\ \ formed}{(unit\ \ time)(unit\ \ NQ)}, \ e.g., \ \frac{\text{mol}}{(\text{s})(\text{m}^3)}$$

Time Quantities

- Thời gian lưu (Resident time) t của một phần tử chất lỏng là thời gian phần tử chất lỏng đó ở trong bình (vessel). Trong một số trường hợp, thời gian lưu giống nhau đối với tất cả các thành phần của chất lỏng, và trong những trường hợp khác có sự phân bố thời gian cư trú (Resident time distribution, RTD)



- Thời gian lưu trung bình (Mean resident time) $\bar{t}$ là thời gian lưu tb của tất cả các phần tử chất lỏng trong một bình chứa

- Thời gian không gian (Space time) $\boldsymbol{\tau}$ chỉ áp dụng cho các dòng chảy, là thời gian cần thiết cho một thể tích cấp liệu (feed volume) chảy bằng thể tích của bình chứa (vessel volume) để tiến hành quá trình của một thể tích lò phản ứng của vật liệu đầu vào được đo ở những điều kiện đầu vào

Dimensions and Units

Table 1.1 SI primary dimensions and their units

Dimension (quantity)	Dimensional formula	Unit	Symbol of unit
length	[L]	meter	m
mass	[M]	kilogram	kg
amount of substance	$[M_m]$	mole	mol
time	[t]	second	s
temperature	[T]	kelvin	K
electric current	[I]	ampere	A
luminous intensity	(not used here)	candela	cd
dimensional constant molar mass	$[M][M_m]^{-1}$	$kg\ mol^{-1}$	symbol M^a

[a] The value is specific to a species.

Table 1.2 Important SI secondary dimensions and their units

Dimension (quantity)	Dimensional formula	Unit	Symbol of unit
area	$[L]^2$	square meter	m^2
volume	$[L]^3$	cubic meter	m^3
force	$[M][L][t]^{-2}$	newton	N
pressure	$[M][L]^{-1}[t]^{-2}$	pascal	Pa($\equiv$ N m^{-2})
energy	$[M][L]^2[t]^{-2}$	joule	J($\equiv$ N m)
molar heat capacity	$[M][L]^2[t]^{-2}[M_m]^{-1}[T]^{-1}$	(no name)	J mol^{-1} K^{-1}

Table 1.3 Commonly used non-SI units

Quantity	Unit	Symbol of unit	Relation to SI unit
volume	liter	L	10^3 cm^3 = 1 dm^3 = 10^{-3} m^3
pressure	bar	bar	10^5 Pa = 100 kPa = 10^{-1} MPa
energy	calorie	cal	4.1840 J
temperature	degree Celsius	°C	T/K = T/°C + 273.15
time	minute	min	60s
	hour	h	3600s

Table 1.1 Basic units

	Time	Length	Mass	Force	Temperature
SI	s	m	kg	–	K, ^{0}C
CGS	s	cm	g	–	K, ^{0}C
US Engineering	s	ft	lb_m	lb_f	^{0}R, ^{0}F

Table 1.2 Derived units

	SI	US Engineering
Force	N (1 N = 1 kg m/s^2)	–
Energy	J (1 J = 1 kg m^2/s^2)	Btu
Power	W (1 W = 1 J/s)	HP, PS
Area	m^2	ft^2
Volume	m^3 (1m^3 = 1000 l)	ft^3
Density	kg/m^3	lb_m/ft^3
Velocity	m/s	ft/s
Pressure	Pa (1 Pa = 1 N/m^2) bar (1 bar = 10^5 Pa) torr (1 torr = 1 mmHg) atm (1 atm = 101325 Pa)	psi = lb_f/in^2

Table 1.3 Conversion factors

1 ft = 12 in = 0.3048 m	$^0F = 32+1.8* {}^0C$
1 in = 2.54 cm	$^0C = (^0F-32)/1.8$
1 US gallon = 3.7854 l	$^0R = 460 + {}^0F$
1 lb_m = 0.4536 kg	$K = 273.15 + {}^0C$
1 lb_f = 4.4482 N	
1 psi = 6894.76 Pa	$\Delta^0C = \Delta^0F/1.8$
1 HP = 745.7 W	$\Delta^0C = \Delta K$
1 Btu = 1055.06 J = 0.25216 kcal	$\Delta^0F = \Delta^0R$
1kWh = 3600 kJ	

Table A.1.1 SI Prefixes

Factor	Prefix	Symbol	Factor	Prefix	Symbol
10^{18}	exa	E	10^{-1}	deci	d
10^{15}	peta	P	10^{-2}	centi	c
10^{12}	tera	T	10^{-3}	milli	m
10^{9}	giga	G	10^{-6}	micro	μ
10^{6}	mega	M	10^{-9}	nano	n
10^{3}	kilo	k	10^{-12}	pico	p
10^{2}	hecto	h	10^{-15}	femto	f
10^{1}	deka	da	10^{-18}	atto	a

Force

1 $lb_f = 4.4482$ N

1 N = 1 kg m/s^2

1 dyne = 1 g cm/s^2 = 10^{-5} kg m/s^2

Heat flow

1 Btu/h = 0.29307 W

1 Btu/min = 17.58 W

1 kJ/h = 2.778×10^{-4} kW

1 J/s = 1 W

Heat flux

1 Btu/(h ft^2) = 3.1546 W/m^2

Heat transfer coefficient

1 Btu/(h ft^2 °F) = 5.6783 W/(m^2 K)

1 Btu/(h ft^2 °F) = 1.3571×10^{-4} cal/(s cm^2 °C)

Length

1 ft = 0.3048 m

1 micron = 10^{-6} m = 1 μm

1 Å = 10^{-10} m

1 in = 2.54×10^{-2} m

1 mile = 1.609344×10^3 m

Mass

1 carat = 2×10^{-4} kg

1 lb_m = 0.45359 kg

1 lb_m = 16 oz = 7000 grains

1 ton (metric) = 1000 kg

Mass transfer coefficient

1 lb mol/(h ft^2 mol fraction) = 1.3562×10^{-3} kg mol/(s m^2 mol fraction)

Acceleration of gravity

$g = 9.80665\ m/s^2$

$g = 980.665\ cm/s^2$

$g = 32.174\ ft/s^2$

$1\ ft/s^2 = 0.304799\ m/s^2$

Area

$1\ acre = 4.046856 \times 10^3\ m^2$

$1\ ft^2 = 0.0929\ m^2$

$1\ in^2 = 6.4516 \times 10^{-4}\ m^2$

Density

$1\ lb_m/ft^3 = 16.0185\ kg/m^3$

$1\ lb_m/gal = 1.198264 \times 10^2\ kg/m^3$

Density of dry air at 0°C, 760 mm Hg = 1.2929 g/L

1 kg mol ideal gas at 0°C, 760 mm Hg = $22.414\ m^3$

Diffusivity

$1\ ft^2/h = 2.581 \times 10^{-5}\ m^2/s$

Energy

1 Btu = 1055 J = 1.055 kJ

1 Btu = 252.16 cal

1 kcal = 4.184 kJ

$1\ J = 1\ N\ m = 1\ kg\ m^2/s^2$

$1\ kW\ h = 3.6 \times 10^3\ kJ$

Enthalpy

$1\ Btu/lb_m = 2.3258\ kJ/kg$

Power

1 hp = 0.7457 kW
1 W = 14.34 cal/min
1 hp = 550 ft lb_f/s
1 Btu/h = 0.29307 W
1 hp = 0.7068 Btu/s
1 J/s = 1 W

Pressure

1 psia = 6.895 kPa
1 psia = 6.895×10^3 N/m^2
1 bar = 1×10^5 Pa = 1×10^5 N/m^2
1 Pa = 1 N/m^2
1 mm Hg (0°C) = 1.333224×10^2 N/m^2
1 atm = 29.921 in. Hg at 0°C
1 atm = 33.90 ft H_2O at 4°C
1 atm = 14.696 psia = 1.01325×10^5 N/m^2
1 atm = 1.01325 bar
1 atm = 760 mm Hg at 0°C = 1.01325×10^5 Pa
1 lb_f/ft^2 = 4.788×10^2 dyne/cm^2 = 47.88 N/m^2

Specific heat

1 Btu/(lb_m °F) = 4.1865 J/(g K)
1 Btu/(lb_m °F) = 1 cal/(g °C)

Temperature

$T_{°F} = T_{°C} \times 1.8 + 32$
$T_{°C} = (T_{°F} - 32)/1.8$

Thermal conductivity

1 Btu/(h ft °F) = 1.731 W/(m K)

1 Btu in/(ft^2 h °F) = 1.442279 × 10^{-2} W/(m K)

Viscosity

1 lb$_m$/(ft h) = 0.4134 cp

1 lb$_m$/(ft s) = 1488.16 cp

1 cp = 10^{-2} g/(cm s) = 10^{-2} poise

1 cp = 10^{-3} Pa s = 10^{-3} kg/(m s) = 10^{-3} N s/m^2

1 lb$_f$ s/ft^2 = 4.7879 × 10^4 cp

1 N s/m^2 = 1 Pa s

1 kg/(m s) = 1 Pa s

Volume

1 ft^3 = 0.02832 m^3

1 U.S. gal = 3.785 × 10^{-3} m^3

1 L = 1000 cm^3

1 m^3 = 1000 L

1 U.S. gal = 4 qt

1 ft^3 = 7.481 U.S. gal

1 British gal = 1.20094 U.S. gal

Work

1 hp h = 0.7457 kW h

1 hp h = 2544.5 Btu

1 ft lb$_f$ = 1.35582 J

Bài tập chương 2

Bài 1: Chuyển đổi những giá trị đơn vị sau

a. 100 Btu/h ft^2 °F thành kW/m^2 °C
b. 100 lb mol/h ft^2 thành kg mol/s m^2
c. 10 ft lb_f/lb_m thành J/kg
d. 0.5 lb_f s/ft^2 thành Pa s
e. 251°F thành °C
f. 0.8 cal/g °C thành J/kg K