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PRESENTATION ON

KINETICS OF EXPLOSIVE REACTIONS

FOR THE SUBJECT

CUTM 1649 MODERN AND APPLIED ANALYTICAL FORENSIC CHEMISTRY

**SCHOOL OF FORENSIC SCIENCES
BHUBANESHWAR CAMPUS**



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**MODERN & APPLIED ANALYTICAL FORENSIC
CHEMISTRY**

Kinetics of explosive reactions

**PRAJNA PARAMITA DASH
212105240011**

**SUBMITTED TO -Dr REENA C .
JHAMTANI**

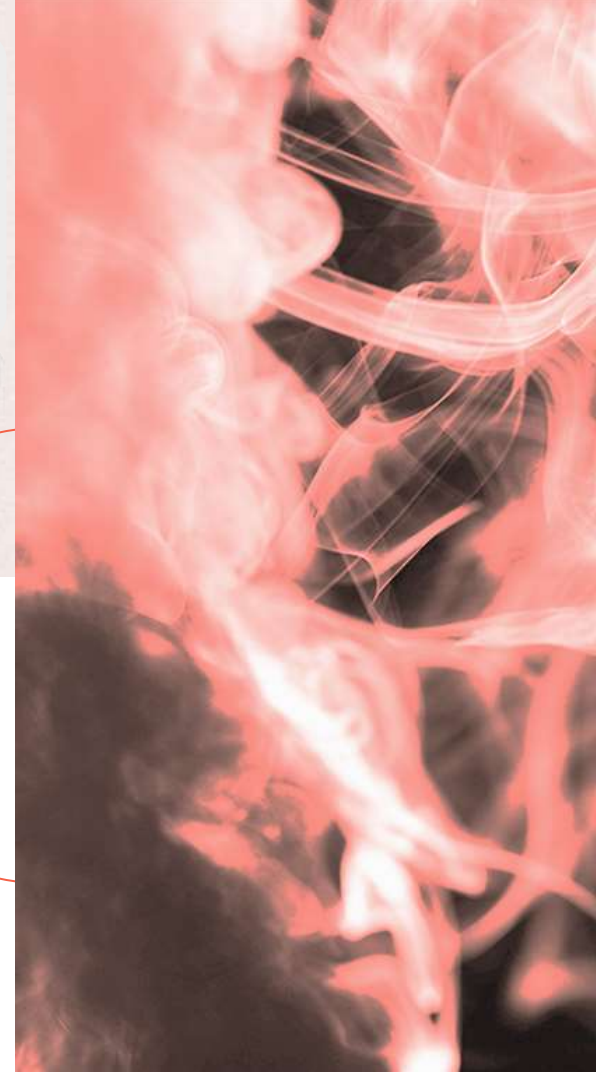


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**DEFLAGRATION &
DETONATION**



Explosive

It is a solid or liquid substance (mixture) which is in itself capable by chemical reaction of producing gas at such a temperature & pressure & at such a speed as to cause damage to the surroundings.

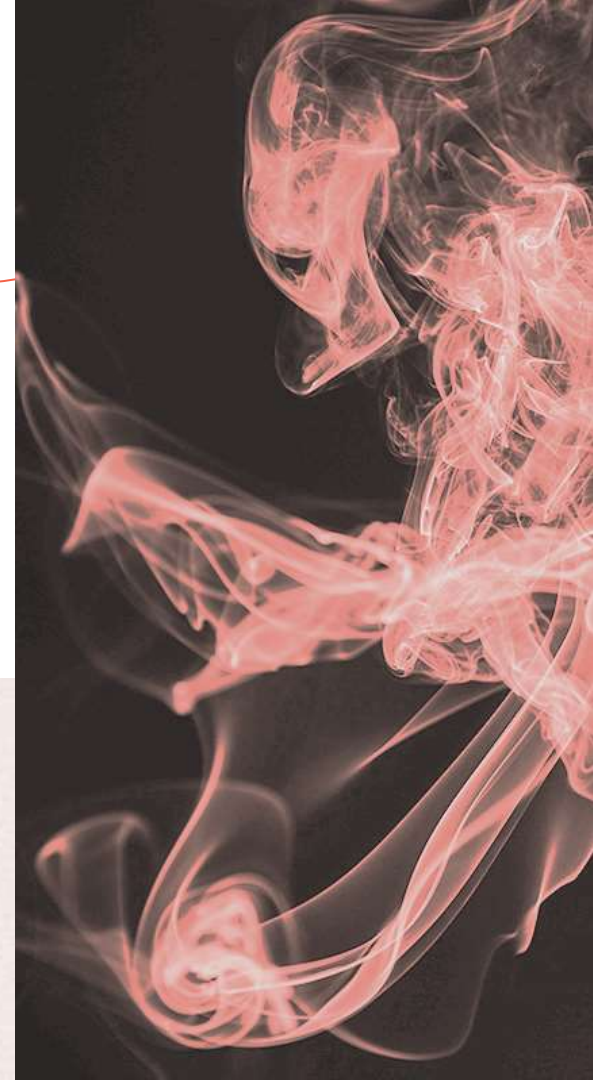
These are sum reactions proceeds explosively either by design or by accident are called as explosion or explosion reaction.

❖ Explosions occur when the rate of one or more steps in a reaction suddenly increases in a very short period of time.

❖ The sudden increase in the rate could be due to autocatalysis (i.e. a radical once produced, goes on producing more radicals of the same type). Often the heat produced in reaction is so large that the container can not accommodate the heat, leading to an explosion.

❖ It is of two types

1. Thermal explosion
2. Chain Branching explosion



Thermal Explosion

- ✓ A thermal explosion is very rapid reaction arising from a rapid increase of reaction rate with increasing temperature
- ✓ Temperature of system rises if the energy released by exothermic reaction & reaction goes faster.

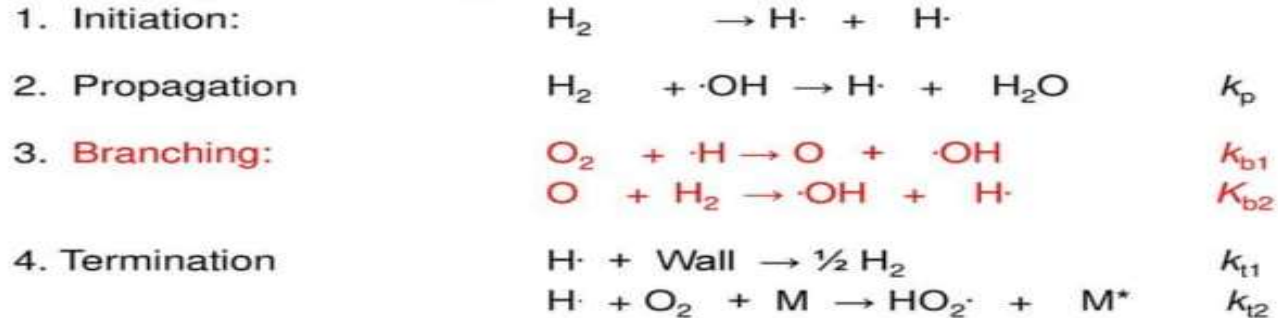
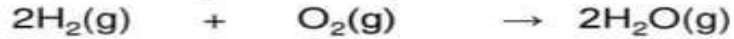
Chain-Branching Explosion

It occurs when the number of chain centres grows exponentially.



Mechanism of Explosive reaction

- An example of both types of explosion is the following reaction



- In last two steps, it can be seen that from each H atoms, two radicals O & H are produce which propagate the chain.
- When reactions proceed to some extent, the amount of free radicals would be very large & an explosion would occur.

- In branching step is elementary reaction that produced more than one chain carries.
- The occurrence of thermal explosion depends upon temperature & pressure of the system.
- At very low pressure the system in outside of explosion are mixture react smoothly at those pressure chain calculated produced in branching step & reach the wall of compound where they combine.
- Rate of formation of radical U_{rad} with $d[H]/dt$
- $U_{rad} = U_{ini} + K_p[OH\cdot][H_2] - K_b[H\cdot][O_2] + K'b[O\cdot][H_2] - K_t[H\cdot] - K't[H\cdot][O_2] [m]$
- Applying steady state approximation to $[OH\cdot]$ & $[O\cdot]$
- $d[OH\cdot]/dt = -K_p[OH\cdot][H_2] + K_b[H\cdot][O_2] + K'b[O\cdot][H_2] = 0$
- $d[O\cdot]/dt = K_b[H\cdot][O_2] - K'b[O\cdot][H_2] = 0$
- Solution of these two algebraic equation are ,
- $[O\cdot] = K_b[H\cdot][O_2] / K'b[H_2]$
- $[OH\cdot] = 2 K_b[H\cdot][O_2] / K_p[H_2]$
- $U_{rad} = U_{ini} + 2K_b[O_2] - K_t - K_t[O_2] [m] [H\cdot]$ we write
- $K_{branch} = 2 K_b [O_2]$ & $K_{term} = K_t + K't [O_2] [H\cdot]$
- $- d[H\cdot]/dt = u_{ini} + (K_{branch} - K_{term}) [H\cdot]$

- When reactions proceed to some extent , the amount of free radicals would be very large and an explosion occur.

- Below a certain pressure , the reaction takes place slowly and smoothly.

- At low pressure the active species or radicals reach the surface easily and gets destroyed.

- The rate of destruction of radicals counter balances the increase of formation of radicals from branching the chain.

- On increasing the pressure , the rate of diffusion of the radicals to the walls decreases and therefore the rate of destruction of radicals also slows down while the rate of propagation and branching increases.

- This due to a considerable rise in concentration of radicals the rate of reaction increases enormously leading to an explosion.

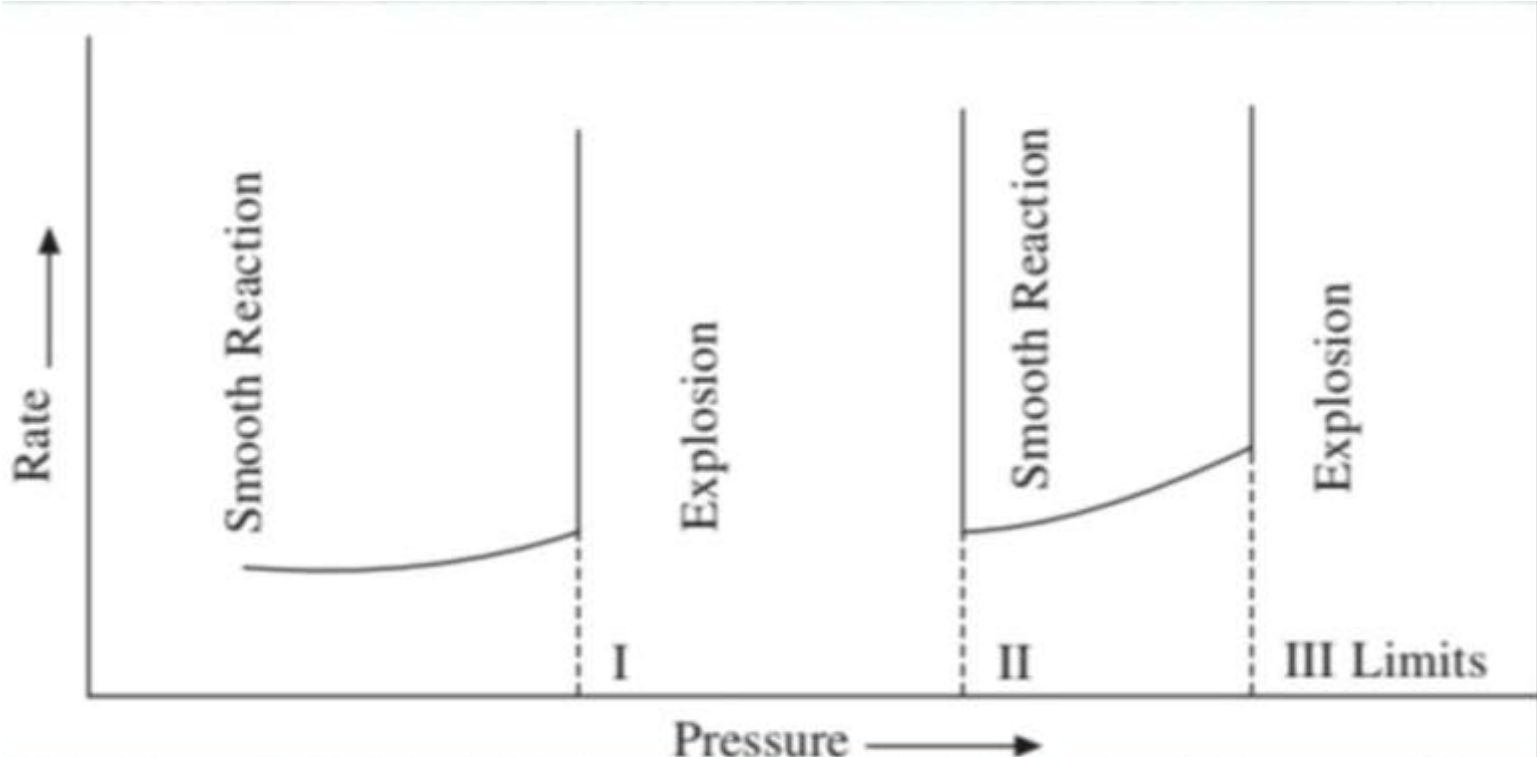
- This is called lower explosion limit.

- On further increasing the pressure , the radicals more readily destroy internally in the gas than at the walls.

- Thus removal of the active species or radicals and any increase in production of radicals is again counter balanced.

- The third limit is due to thermal explosion.

- The reaction rate suddenly becomes very rapid and a thermal explosion occurs.



EXPLOSION IN BRANCHING CHAIN REACTION

Steps in Explosive Reaction

- ❖ This exothermic reaction yields 232 kJ/mol of water formed. The rapid release of a considerable amount of energy causes the surrounding air to expand suddenly, resulting in a sharp explosion.
- ❖ When pure hydrogen is ignited, the reaction with the surrounding air is less rapid, the sound is less loud & a significantly larger flame is produced.
- ❖ Sometimes the chain reaction possesses very high speed which may lead to high explosion.

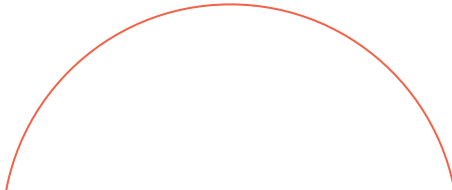
Explosive Chemicals

- Explosives are substances that undergo a rapid oxidation reaction with the production of large quantities of gases.
- Charcoal + potassium Nitrate + Sulphur = Gun powder
- Dynamite & TNT





Combustion

- It is a rapid chemical combination of a substance with oxygen , involving the production of heat & light.
 - It is also defined as the process of burning something.
 - It is a process by which energy is released . This energy is released in two ways which are given as follows:- deflagration
Detonation
- 

Deflagration

- Deflagration is a very rapid oxidation reaction accompanied by generation of (subsonic – slower than the speed of sound) low – intensity pressure wave that can disrupt the surroundings.
- This is caused by the acceleration due to gradual heating up or by the increased pressure of the gases produced by decomposition of the mass according to the conditions prevailing in the explosive system.
- Examples include :-
 1. Internal combustion engine (used in any vehicle that uses fossil fuels such as gasoline , oil or diesel fuel)
 2. Gas stove (natural gas)
 3. Fireworks
 4. Gun powder in a firearm



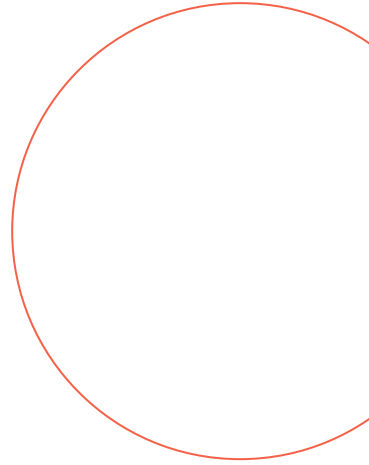
Detonation

- Detonation is an extremely rapid oxidation reaction accompanied by a violent disruptive effect & an intense high speed shockwave (supersonic – faster than the speed of sound) this shockwave breaks the chemical bonds of explosive charge leading to new instantaneous build-up of heat & gases.
- The word “detonation” means “to thunder down” or explode.
- Examples of chemicals that produce detonations include any high explosives , such as:
 - TNT
 - nitroglycerine
 - dynamite
 - picric acid



SIGNIFICANCE

- Assessing the purity
- The uniformity of composition
- point of origin
- Substance involved
- Charge mass
- identification of residues



REFERENCE

<https://slideplayer.com/slide/13503696/>
www.saavyforensic.com
Kinetics of chemistry book

**THANK
YOU**