



B.PHARMA SEM-3

UNIT - 4

PART-1

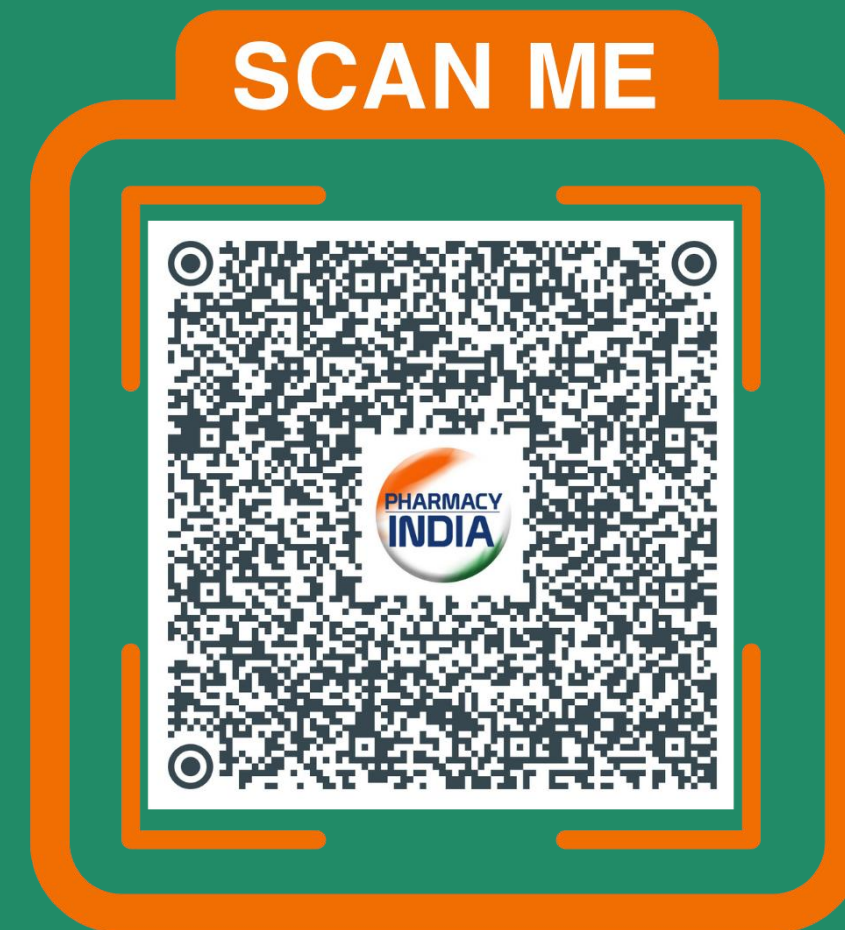
PHARMACEUTICAL ORGANIC CHEMISTRY II

POLYNUCLEAR HYDROCARBONS

INTRODUCTION

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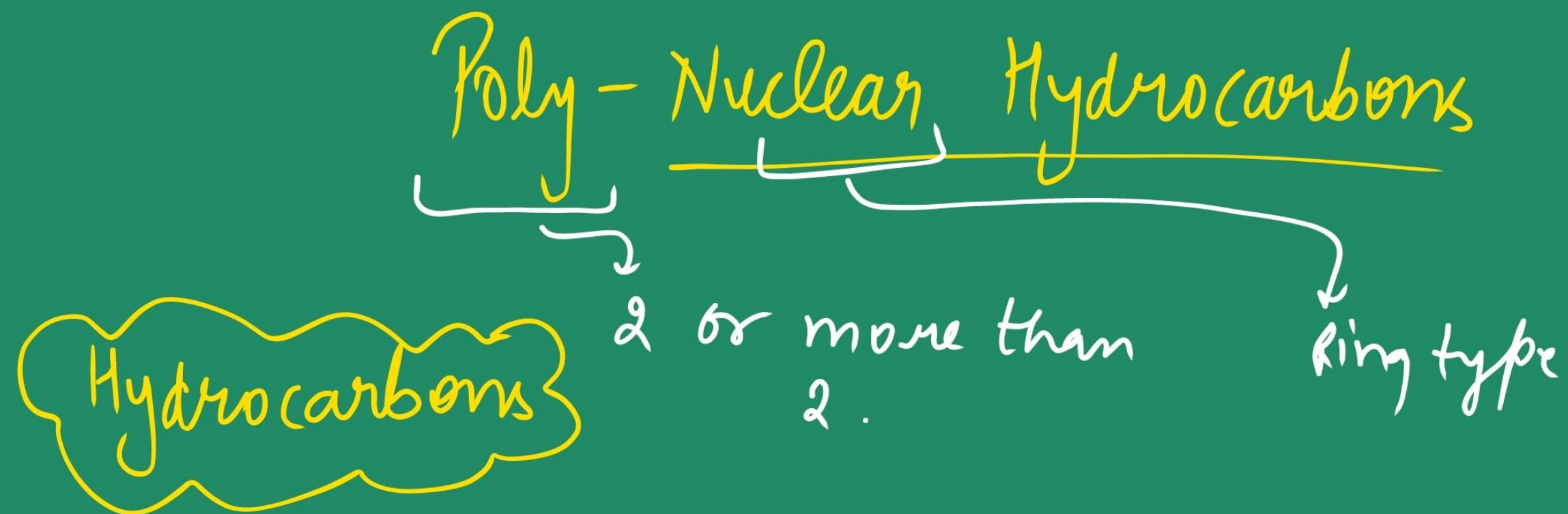


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SEM-3

UNIT-4

TOPIC: Poly-Nuclear Hydrocarbons



Hydrogen + Carbon

The compounds which are made up of Hydrogen & Carbon are called as Hydrocarbon.

eg:- CH_4 , C_2H_6 etc.

Poly + Nuclear

Multiple Rings Hydrocarbons.

Poly nuclear hydrocarbons are the organic compounds which contains only C & H which further composes in the form of Multiple aromatic rings.

eg:- Naphthalene, Anthracene etc.
Phenanthrene.

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PHARMACEUTICAL ORGANIC CHEMISTRY II

POLYNUCLEAR HYDROCARBONS

NAPHTHALENE

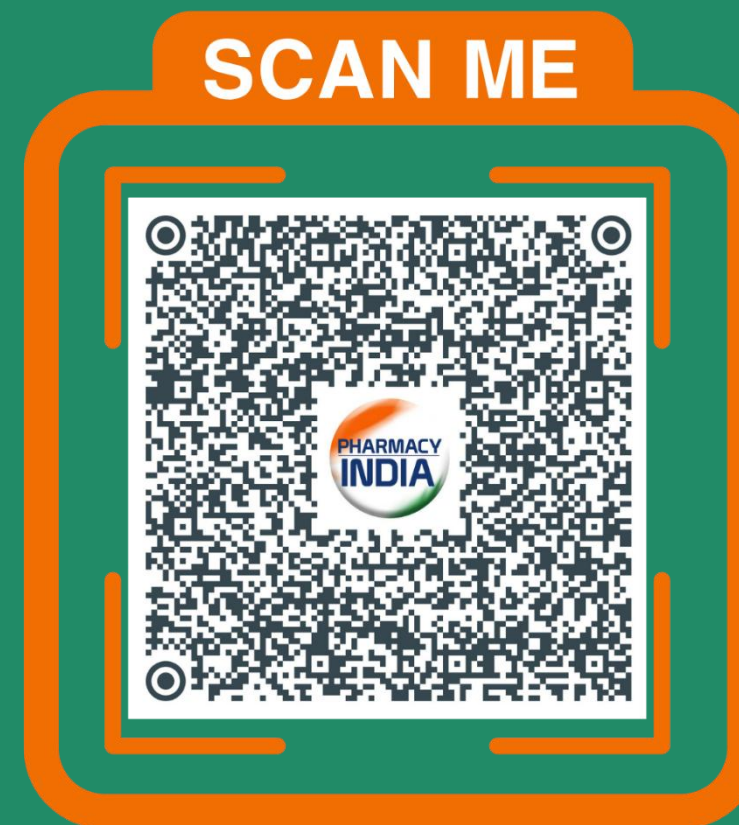
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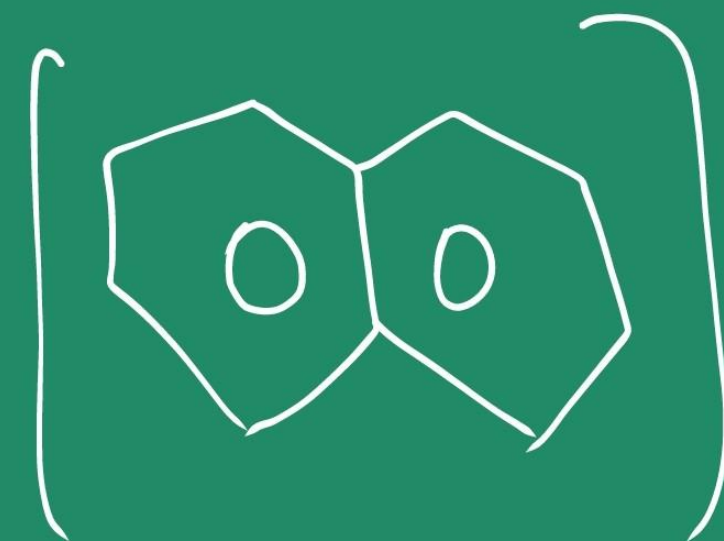
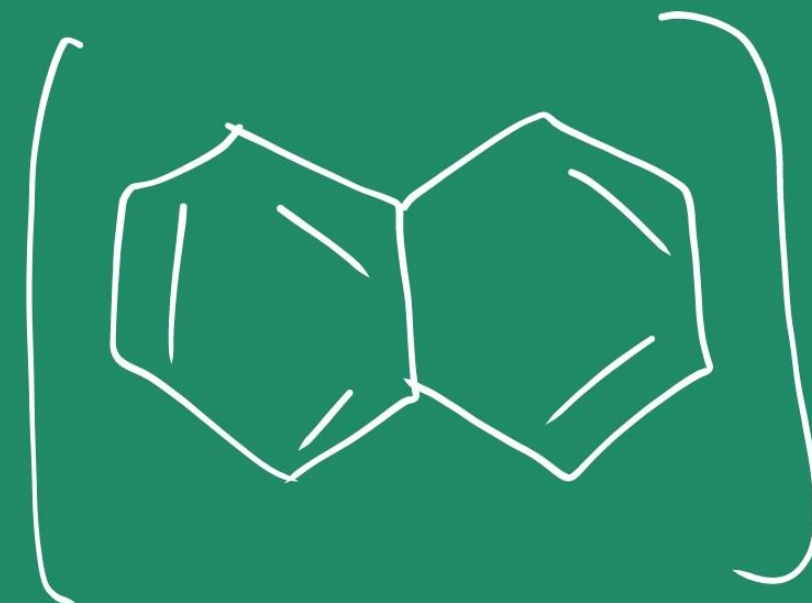
Nepthalene

It is a Polynuclear hydrocarbon.

It's structure is as follows;

Napthalene can also be drawn

as follows;



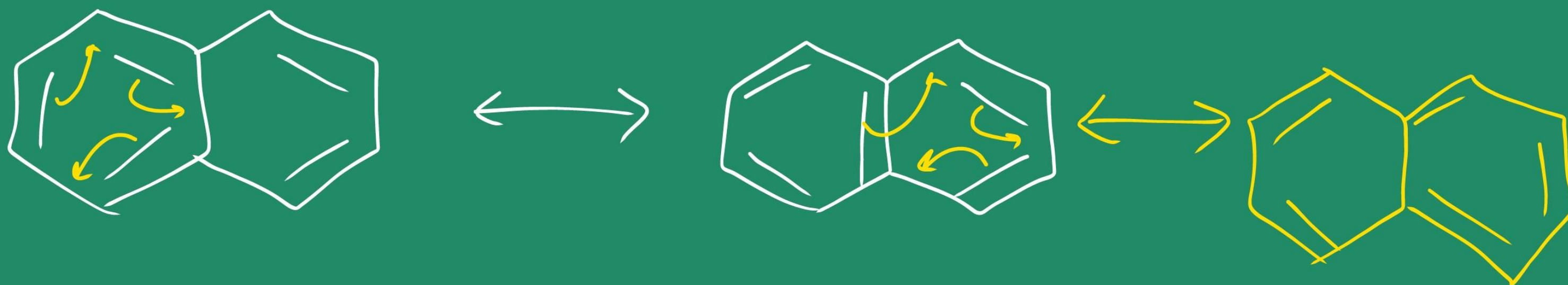
→ It is sp^2 hybridized.

→ Bond Angle: $\sim 120^\circ$

→ C-C; sp^2-sp^2

→ C-H; sp^2-s

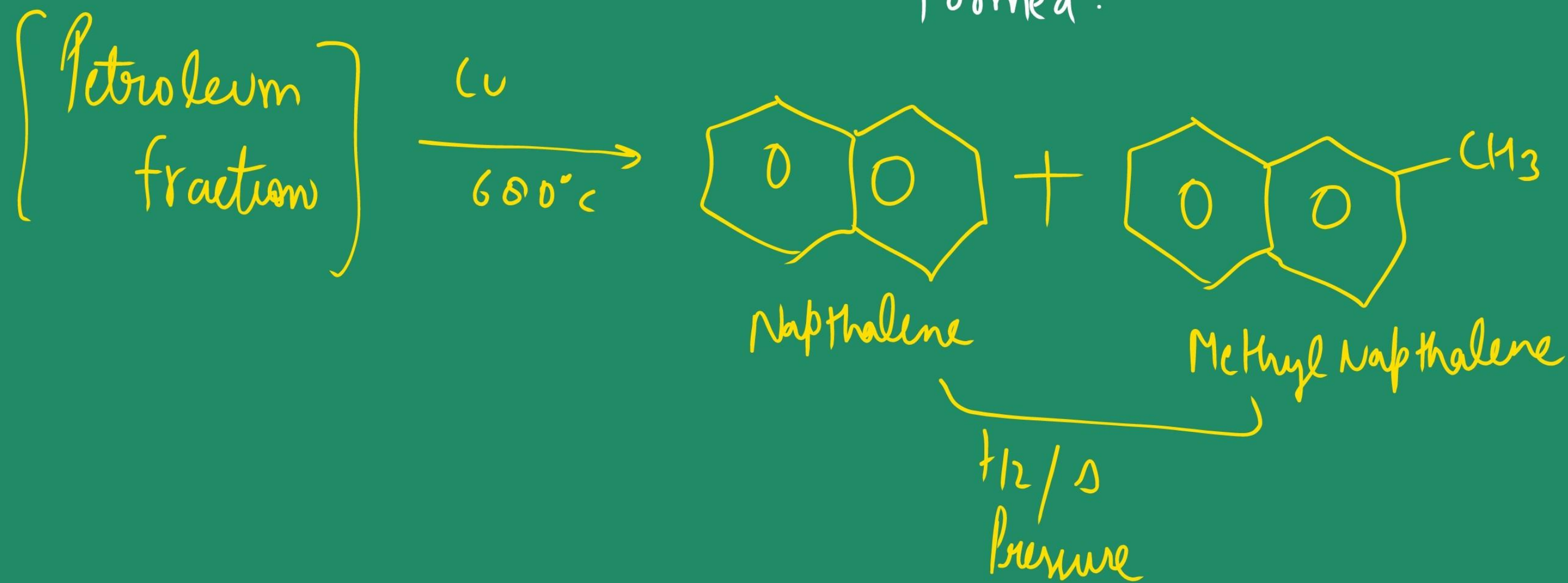
Resonance



There are the Resonating structures.
Bond lengths are different here.

Synthesis

1. From Petroleum: It is fused in the presence of a Cu -catalyst at 600°C ; Naphthalene & Methyl Naphthalene are formed.



Methyl Naphthalene is further separated & converted into Naphthalene.

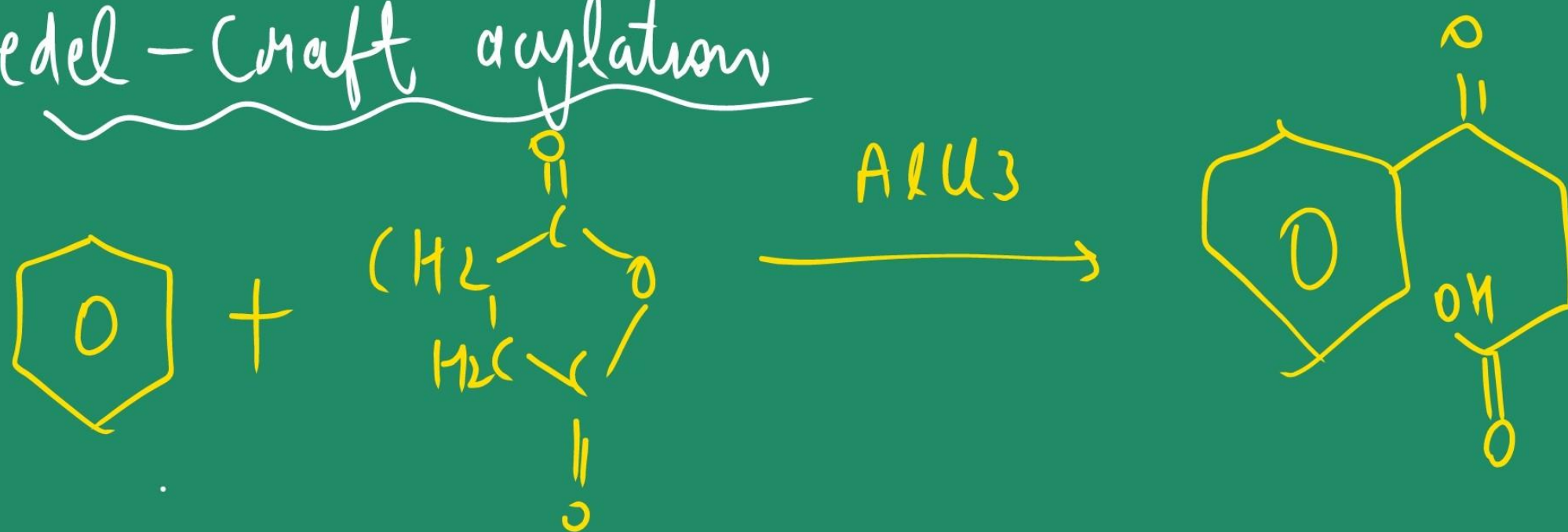
This reaction is also called as de-alkylation.

2.

By Haworth Synthesis

This reaction contains five-steps.

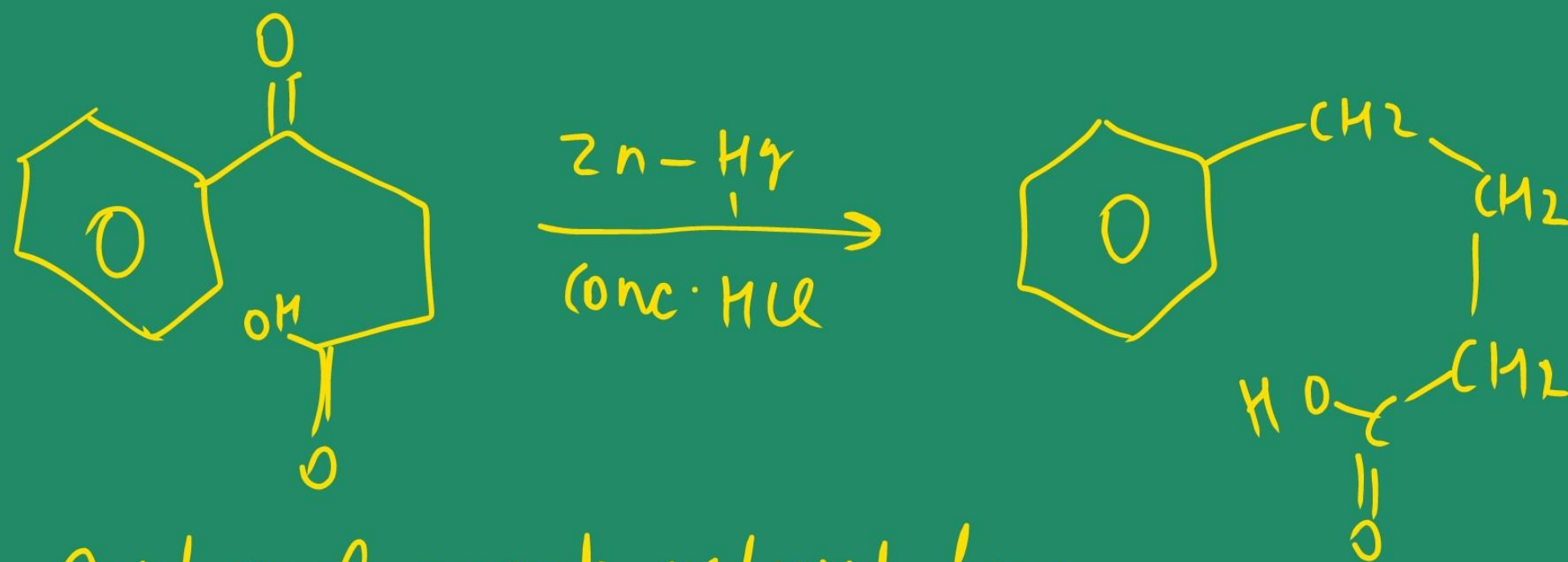
A) Friedel-Craft acylation



Benzene & succinic anhydride are heated in the presence of a lewis acid to form β -Benzyl Propionic acid.

Step. 2

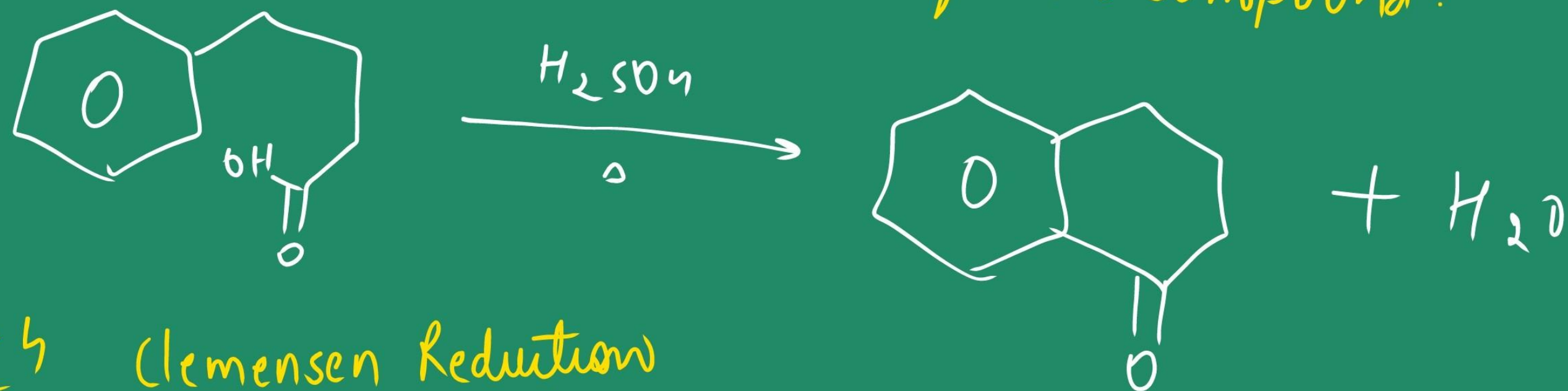
Clemmensen Reduction



Carbonyl group reduced here.

Step 3 Ring closure

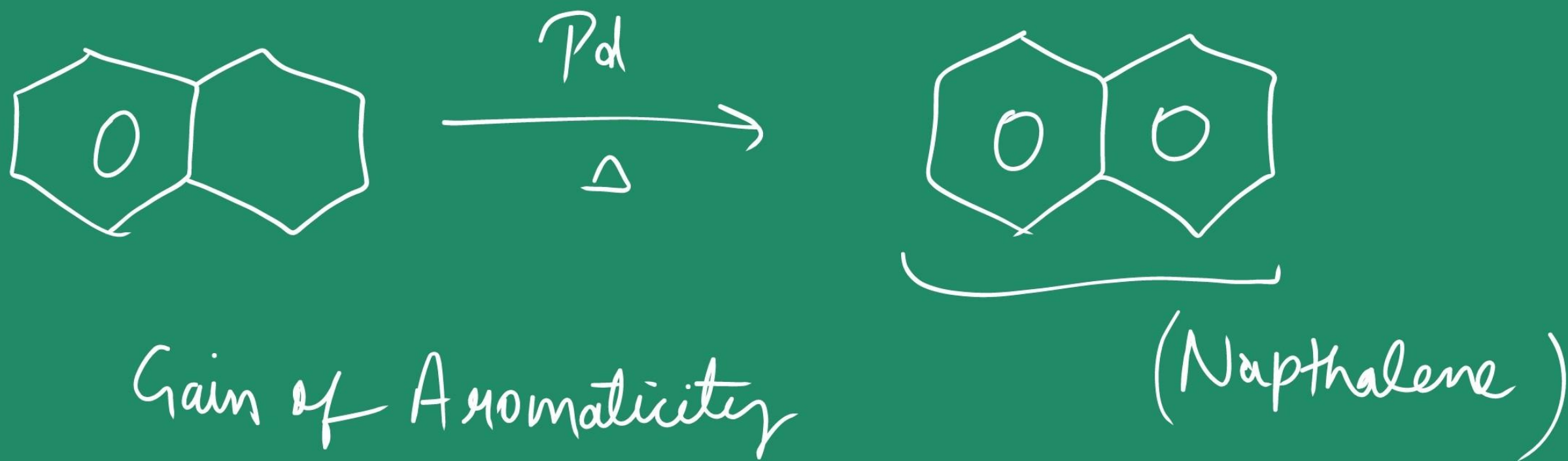
The Product is further heated in the Presence of conc. H_2SO_4 for the formation of new compound.



Step 4 Clemensen Reduction



Step 5 Aromatization Reaction



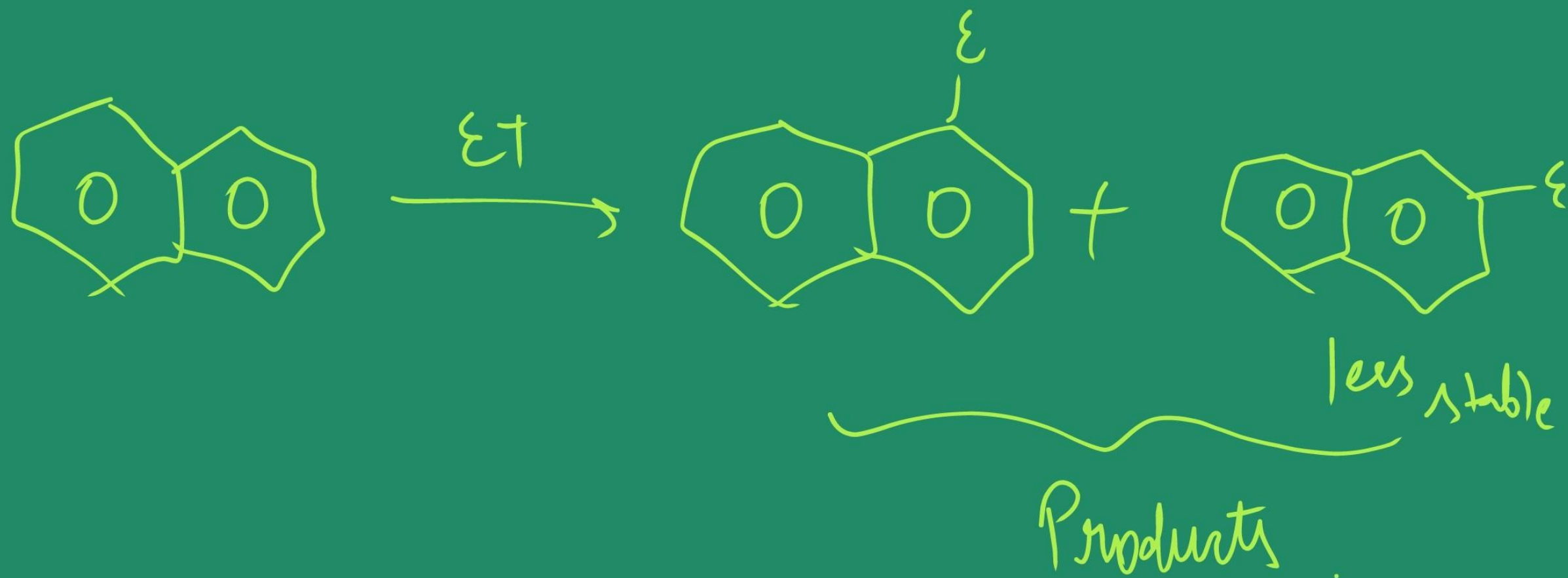
Physical Properties

1. It is a colourless crystalline solid.
2. It is insoluble in water but completely soluble
in organic solvents.
3. It has a characteristic odour.

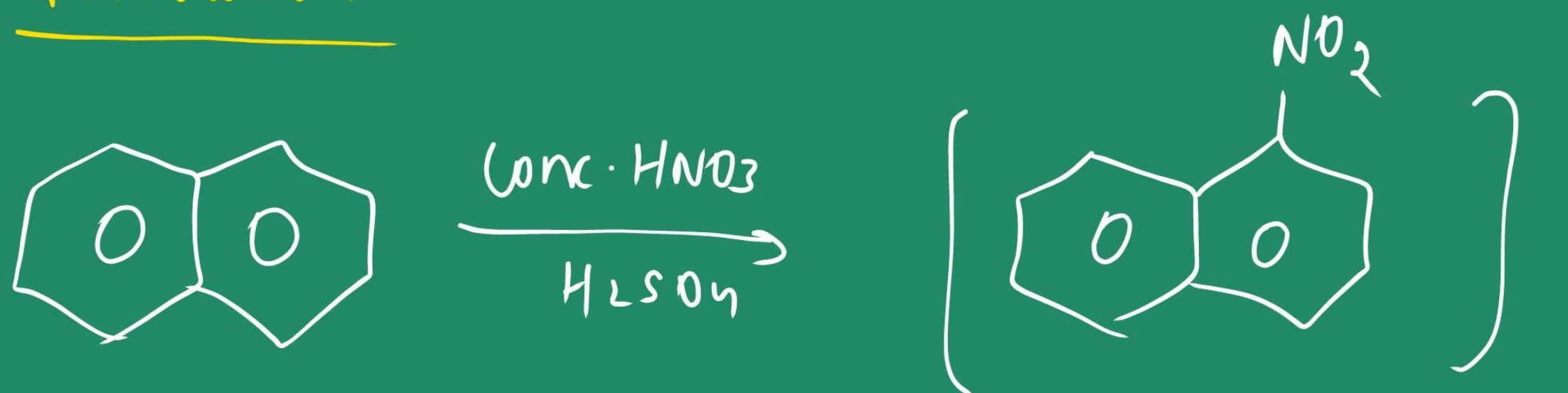
Chemical Properties

Naphthalene shows, Electrophilic substitution Reaction

E^+ attacks on two different Positions & forms the Product.

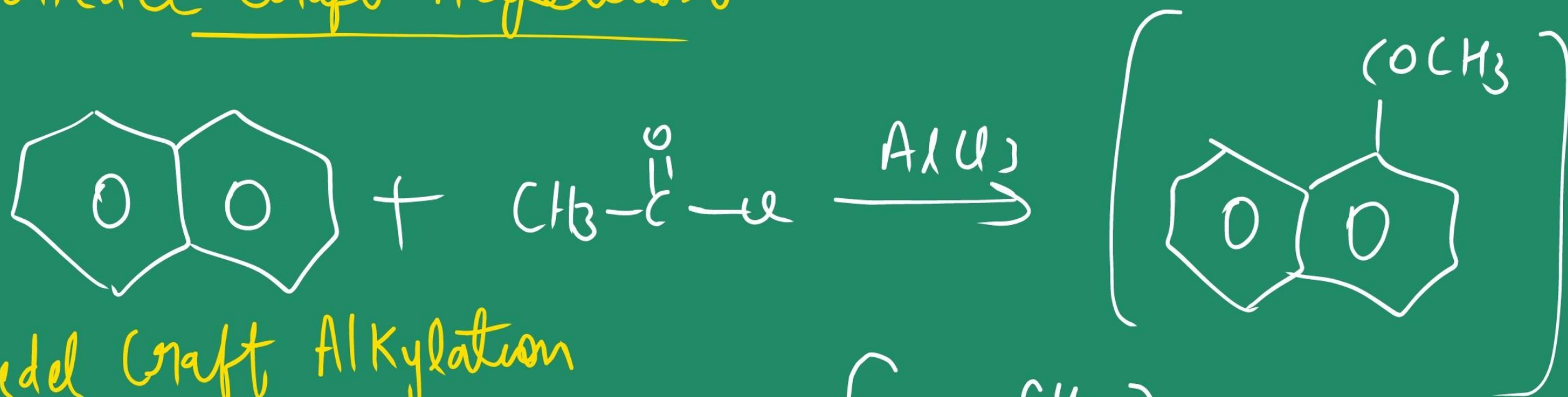


1. Nitration

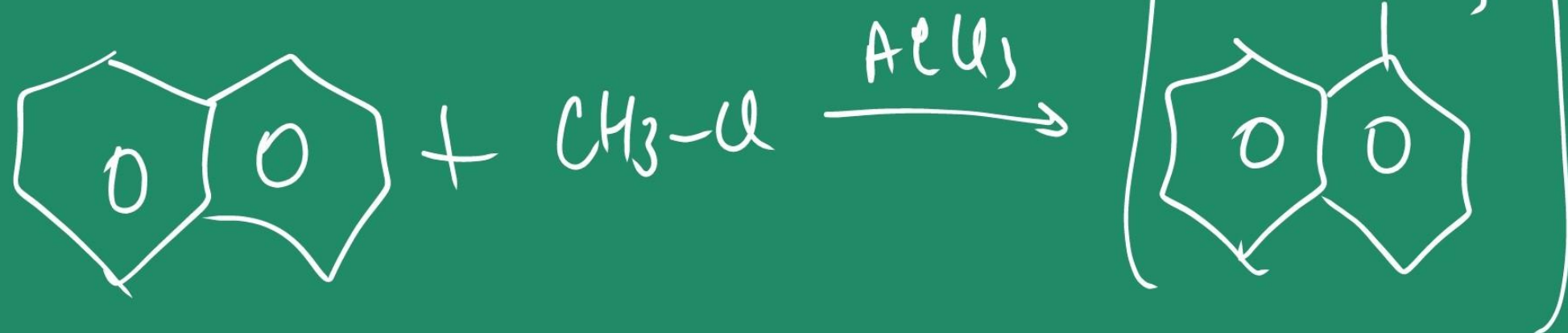


Major Product

2. Friedel Craft Acylation



3. Friedel Craft Alkylation



Medicinal Uses

1. Used in the formation of Methyl balls.
2. Used in the formation of Phthalic anhydride.
3. Used in formation of many medical Products & dyes.

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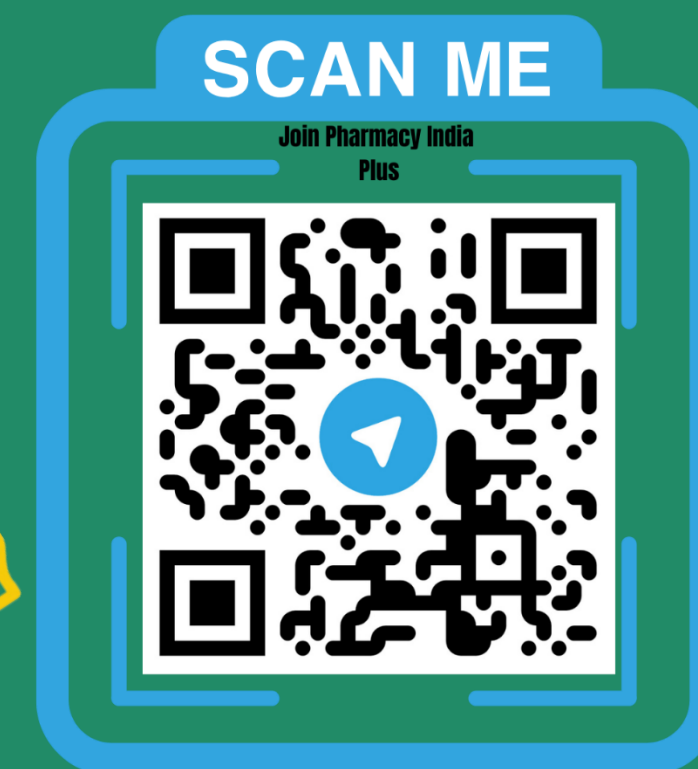
POLYNUCLEAR HYDROCARBONS

PHENANTHRENE

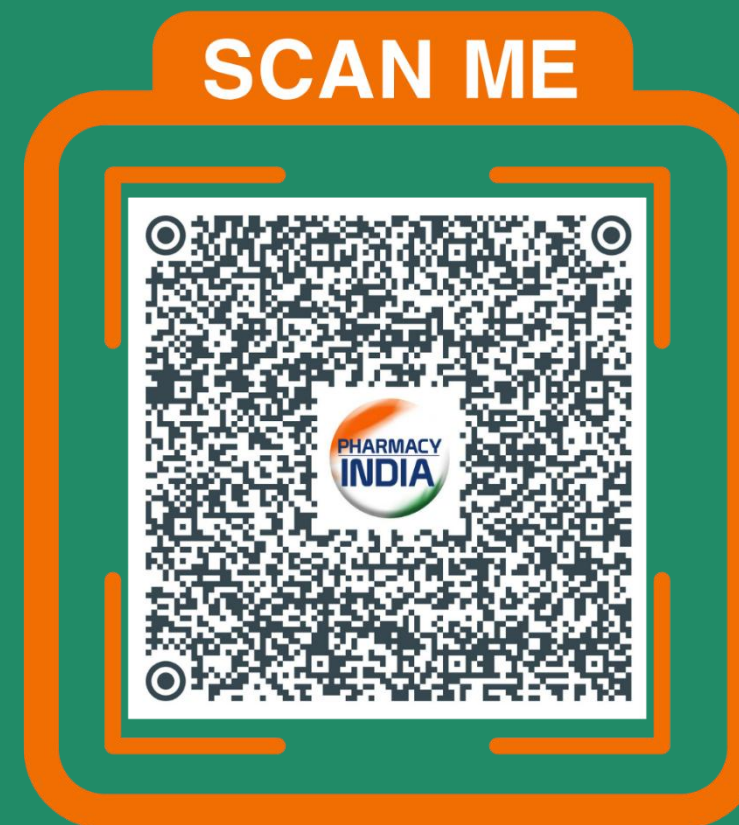
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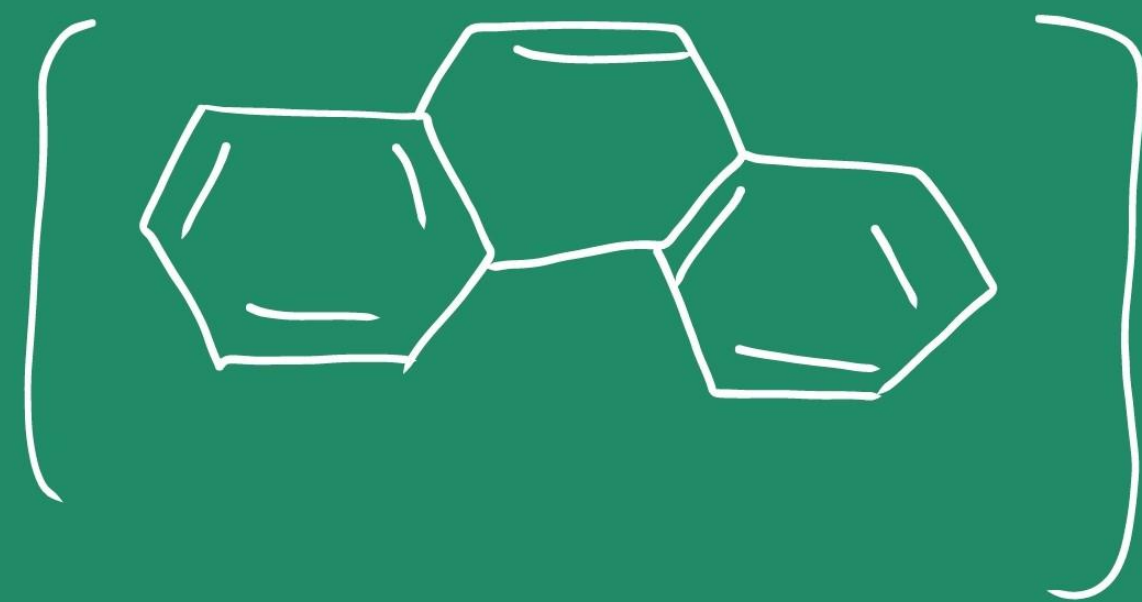
UNIT-4

TOPIC: *Phenanthrene*

/

Phenanthrene

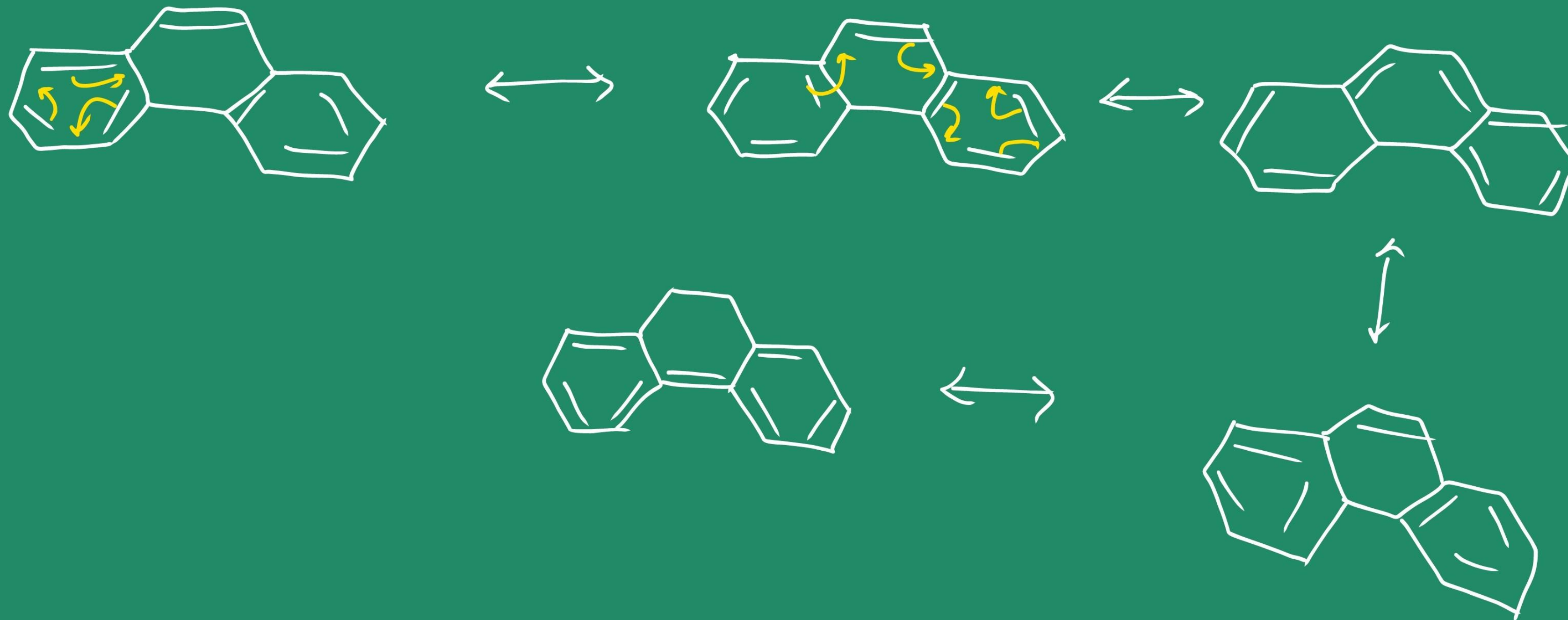
In Phenanthrene, all C-atoms are sp^2 -hybridized.



It is a Polycyclic aromatic compound, this hydrocarbon is made up of three fused Benzene rings.

This is an isomer of Anthracene.

Resonance



Synthesis of Phenanthrene

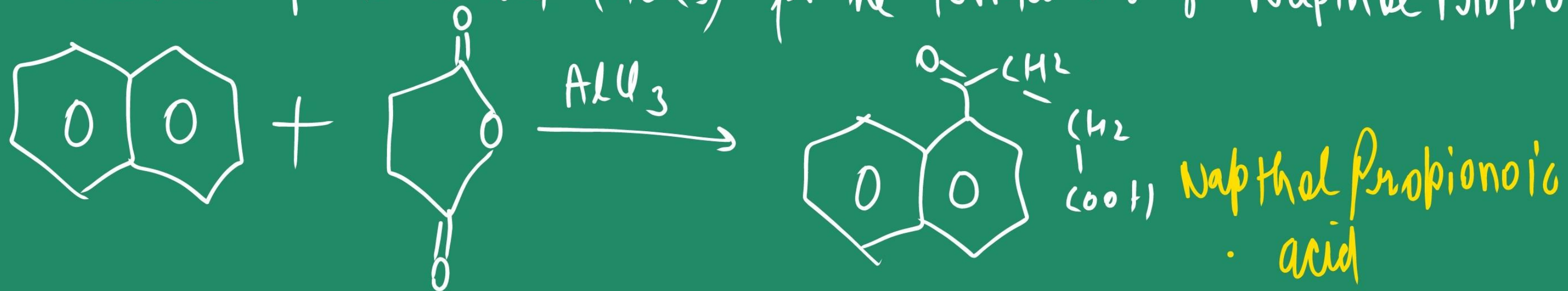
There are many methods for the Preparation of Phenanthrene.

Which are as follows;

1. Haworth Synthesis It contains five steps.

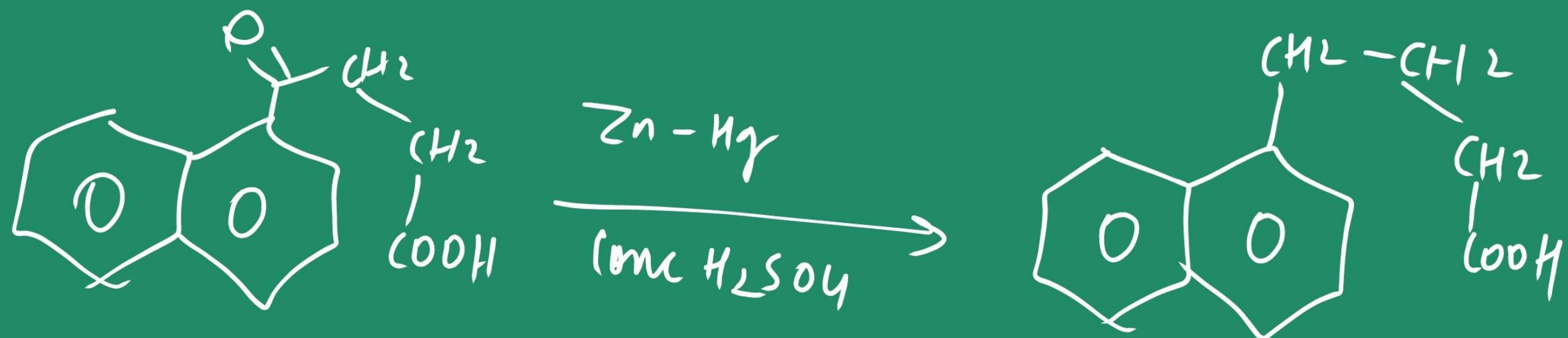
→ Friedel-Craft Acylation

It involves the reaction of Naphthalene with Succinic anhydride in the Presence of Lewis acid ($AlCl_3$) for the formation of Naphthal Propionic acid.

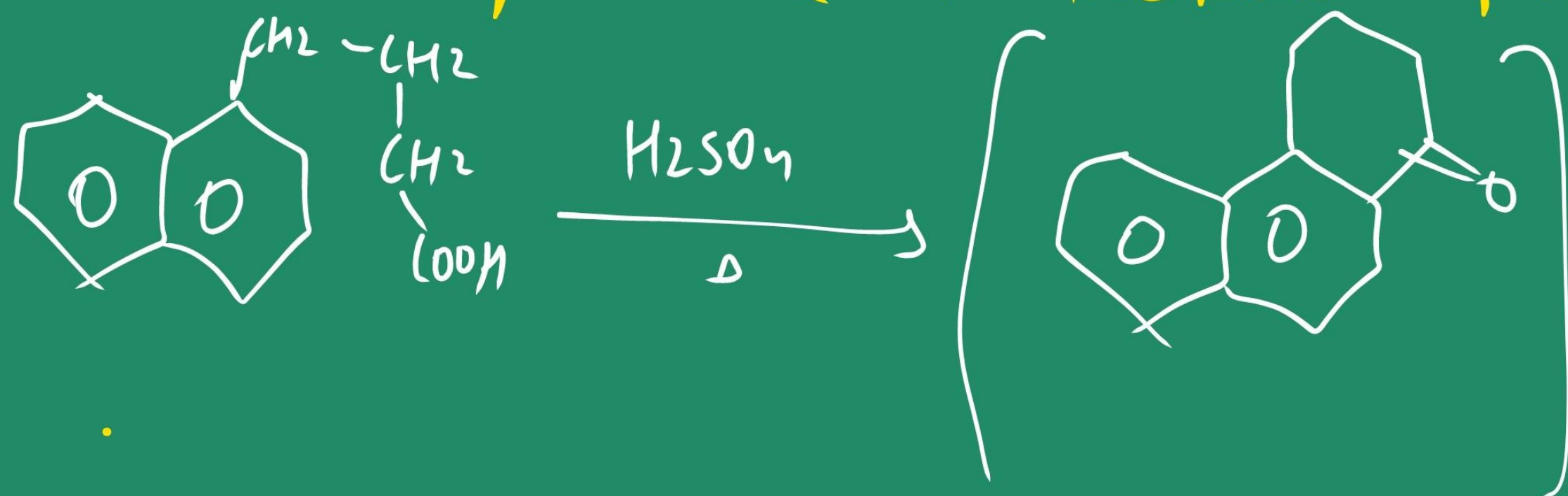


2. Clemmensen Reduction

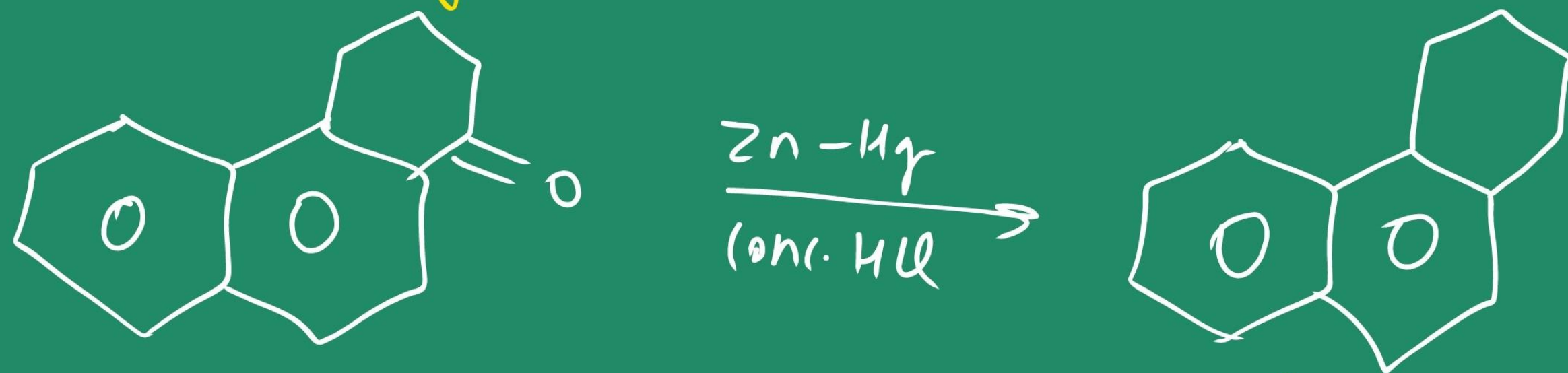
Naphthalenepropanoic acid reacts with amalgamated zinc, in acidic medium.



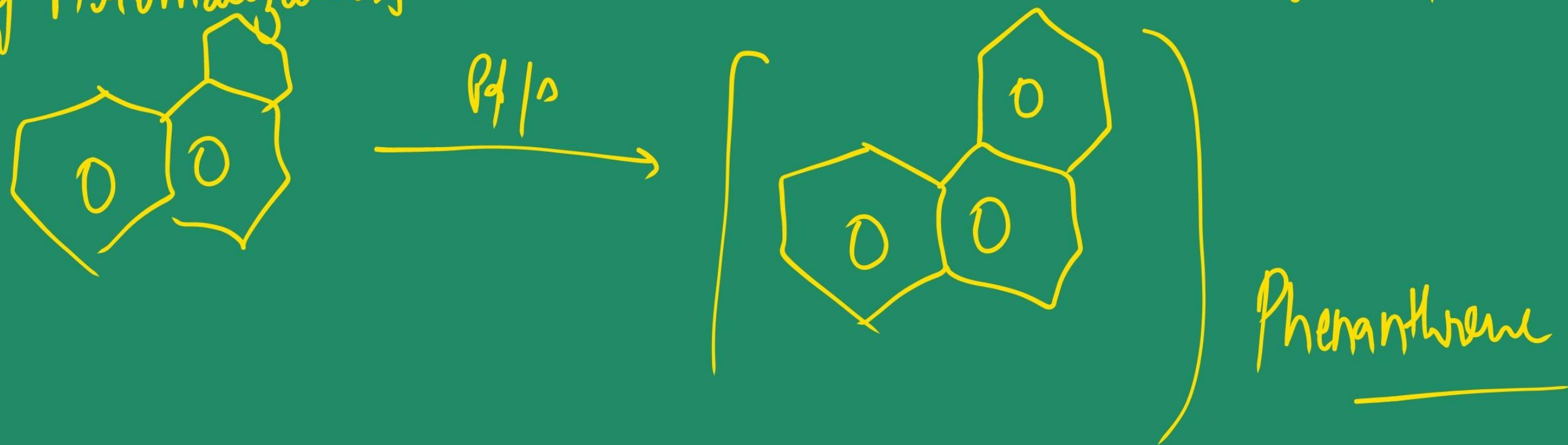
Now, on reacting with H₂SO₄ in the presence of heat, ring closure takes place.



Now, Again applying Clemmensen reduction for the removal of Carbonyl group.

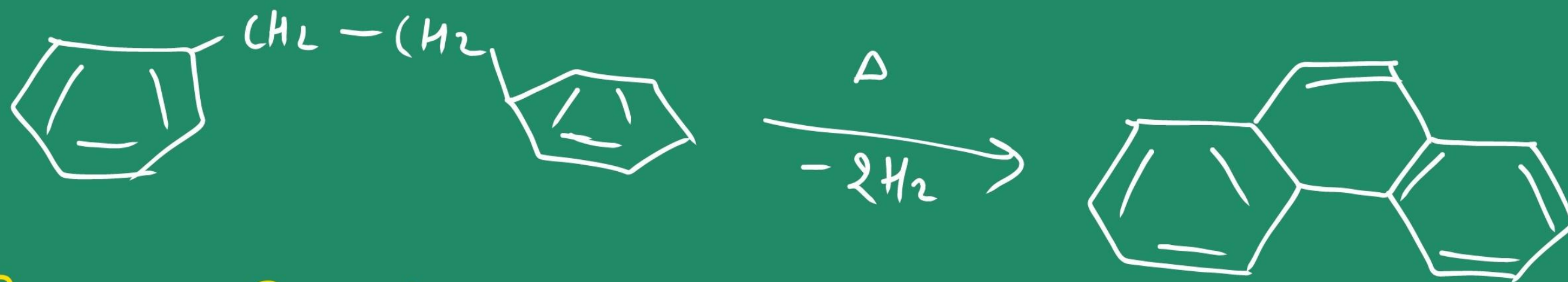


Ring Aromatization will take place in the presence of Pd/ Δ



2. From di-benzyl

Phenanthrene can be obtained on passing di-benzyl to red hot tube.



Physical Properties

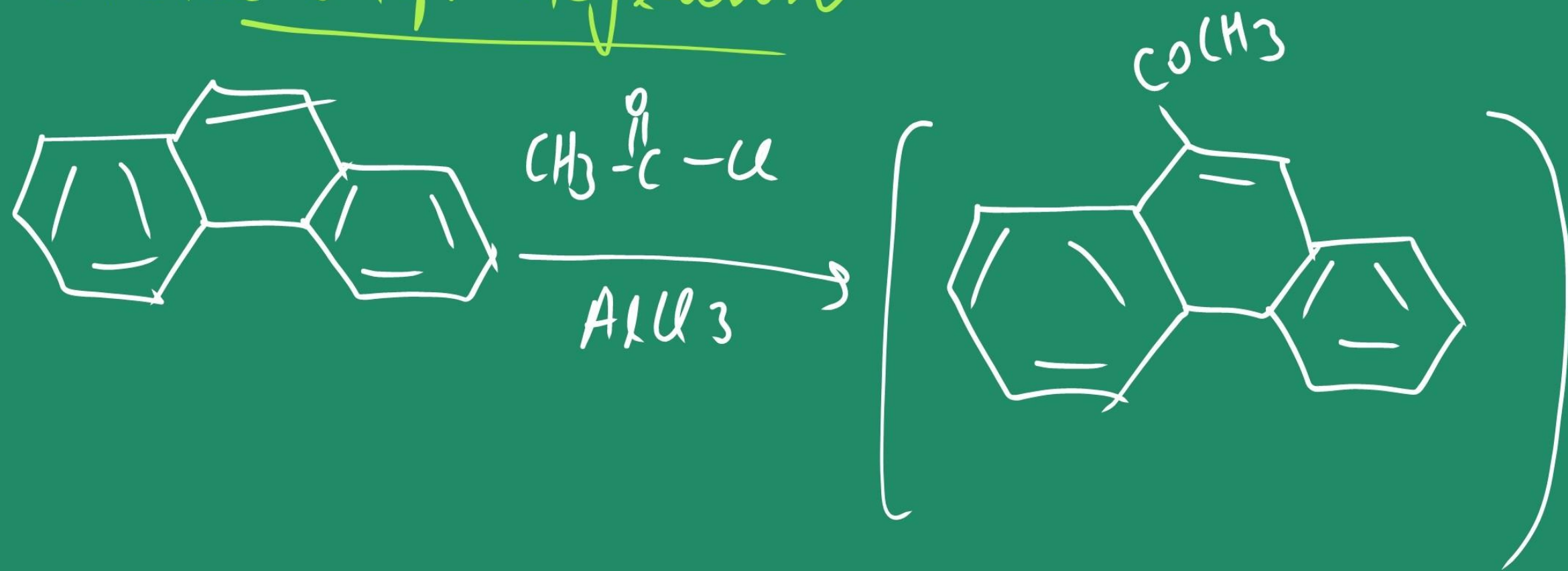
- It is a colourless solid.
- It's melting point is 100°C .
- Insoluble in water but completely soluble in organic comp.

Chemical Properties

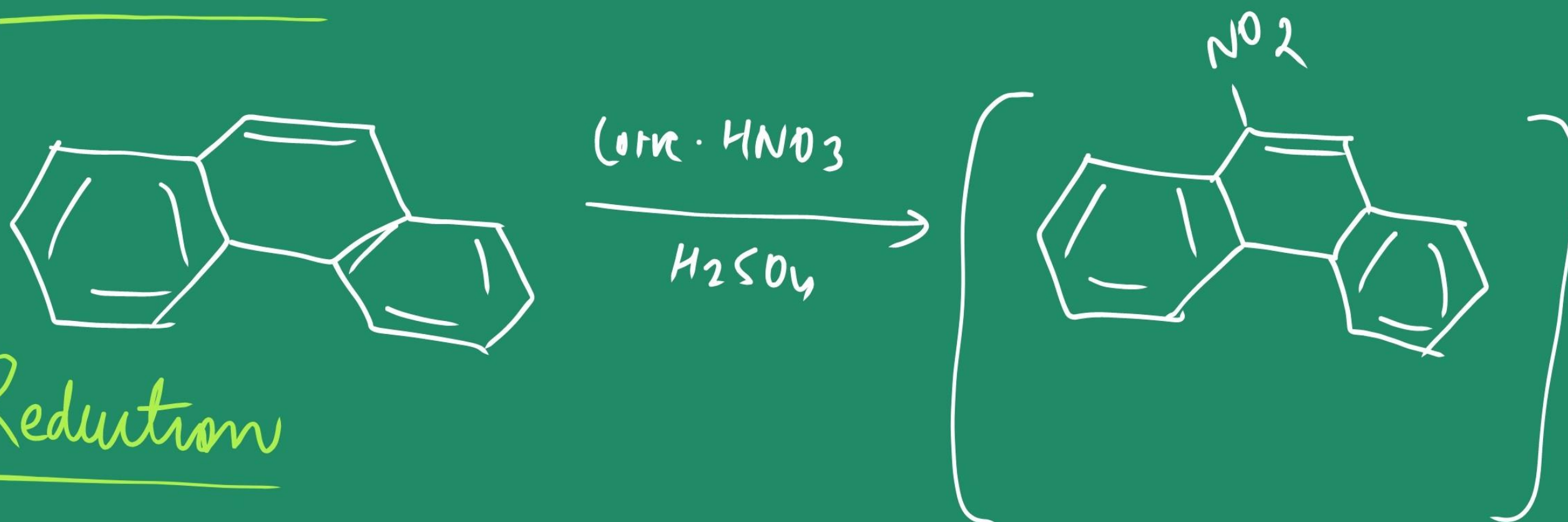
It undergoes Electrophilic substitution reaction, oxidation &

Reduction.

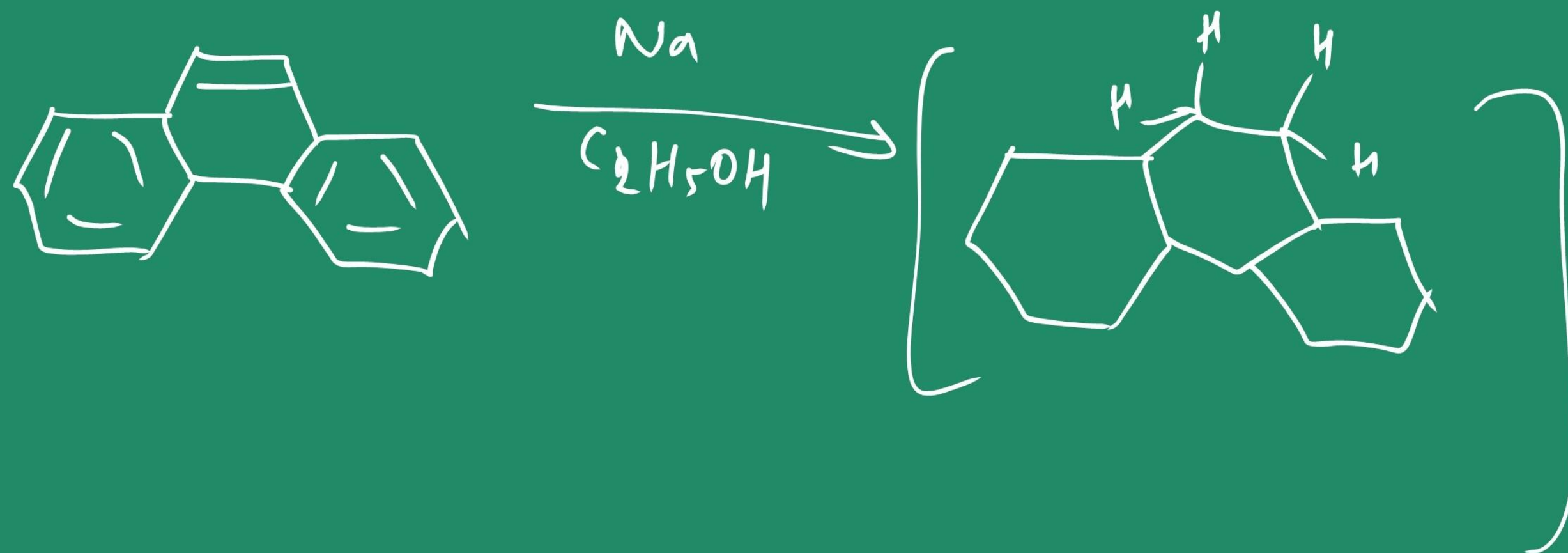
Friedel Craft Acylation



2. Nitration



3. Reduction



Medicinal Uses

1. It is used in the formation of dyes, Plastics & Pesticides.
2. Used in the formation of drugs.
3. Formation of Steroids.



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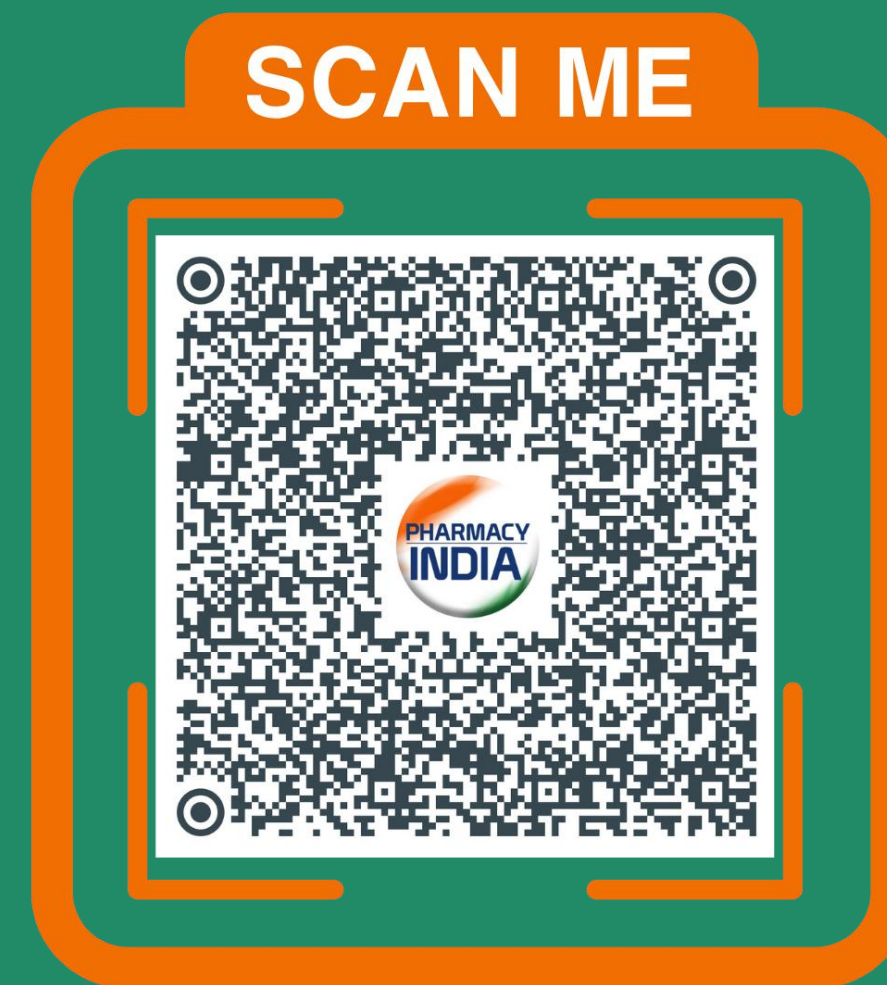
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ANTHRACENE

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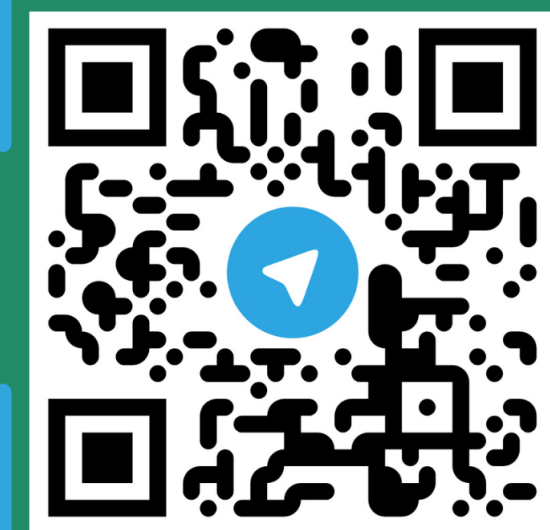
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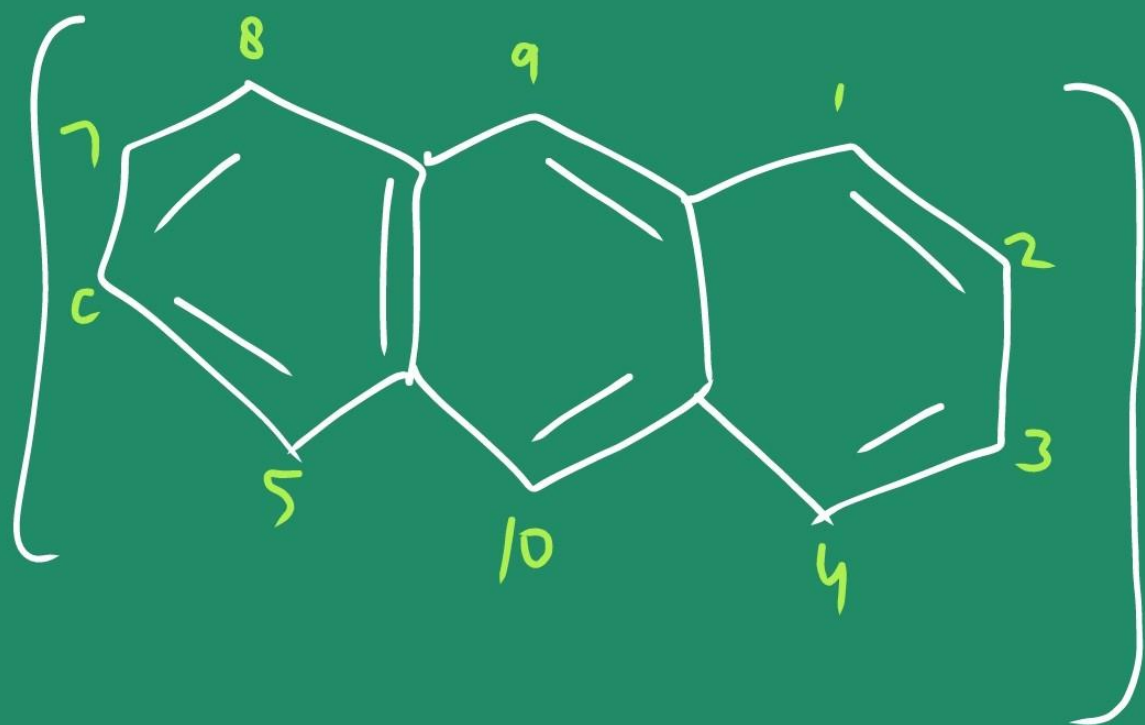
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TOPIC:- Anthracene

Anthracene

It is a Poly-nuclear hydrocarbon which is made up of fusing three Benzene rings.

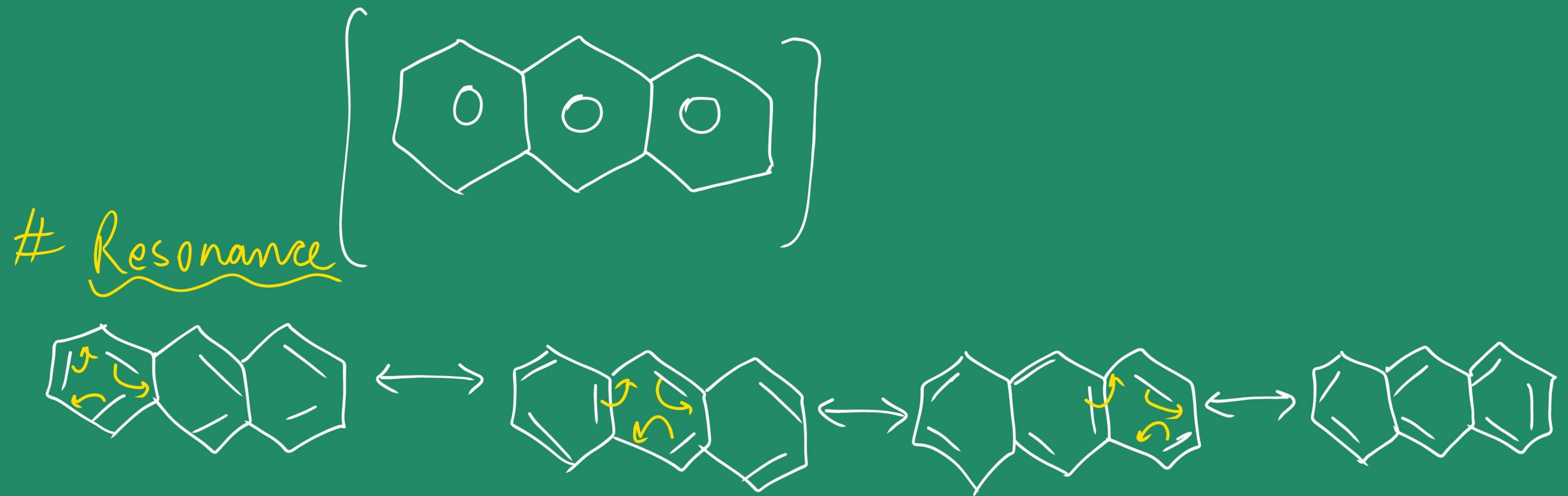


All C-atoms are sp^2 hybridized.

$C=C$: sp^2-sp^2

$C-H$; sp^2-s

The common representation of Anthracene is as follows;

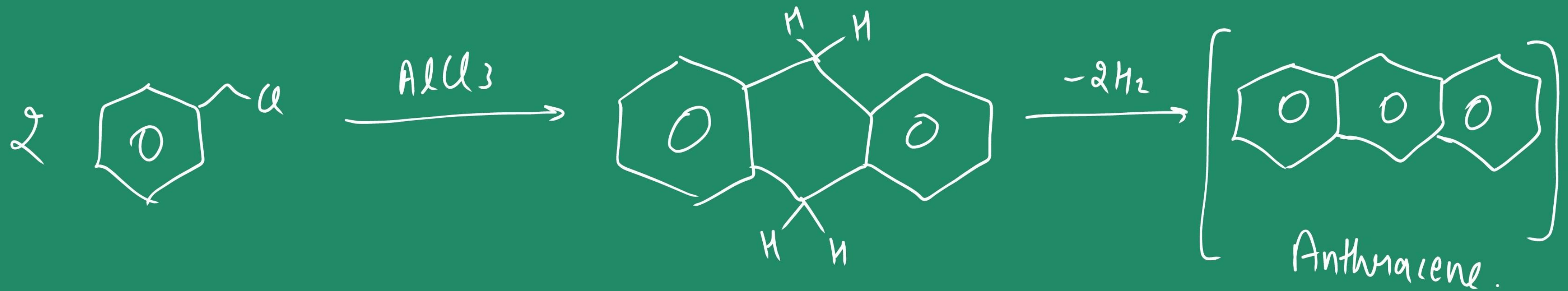


- There are different bond lengths of each C-C atoms.
- The resonance energy of Anthracene is 84 Kcal/mol .

Anthracene is less aromatic compound than Benzene.

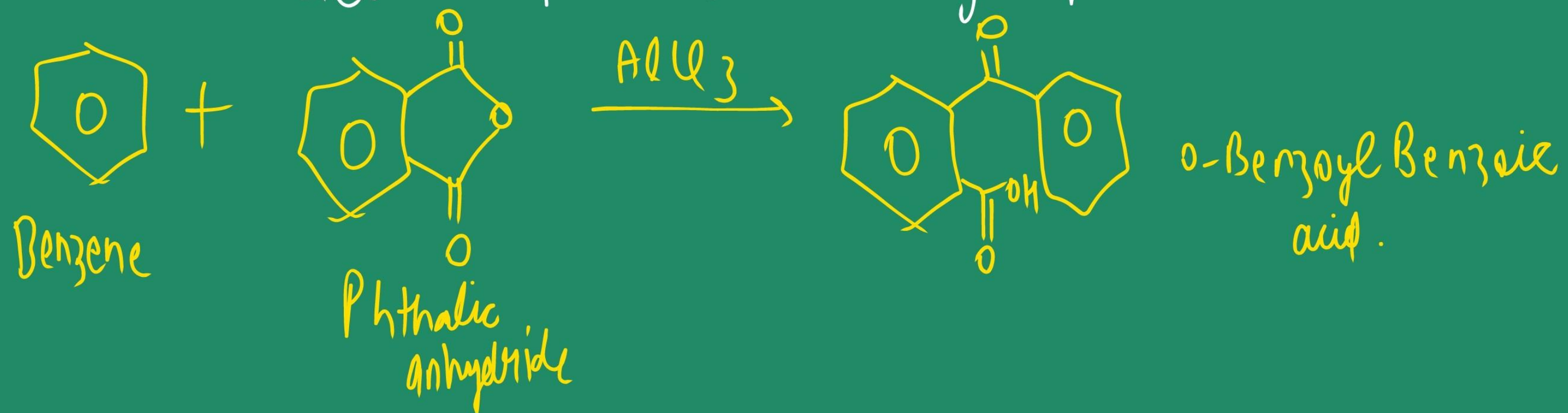
Synthesis

By Friedel Craft Reaction — In this reaction, two compounds of Benzoyl chloride in the presence of Lewis acid to form 9,10 dihydroanthracene. which readily loses hydrogen & convert into Anthracene.

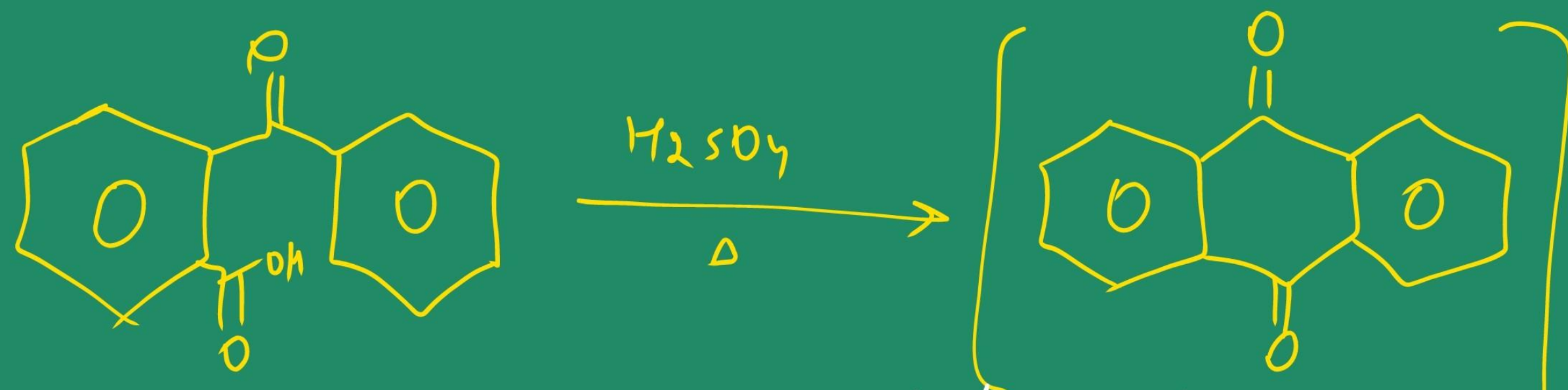


By Haworth Synthesis

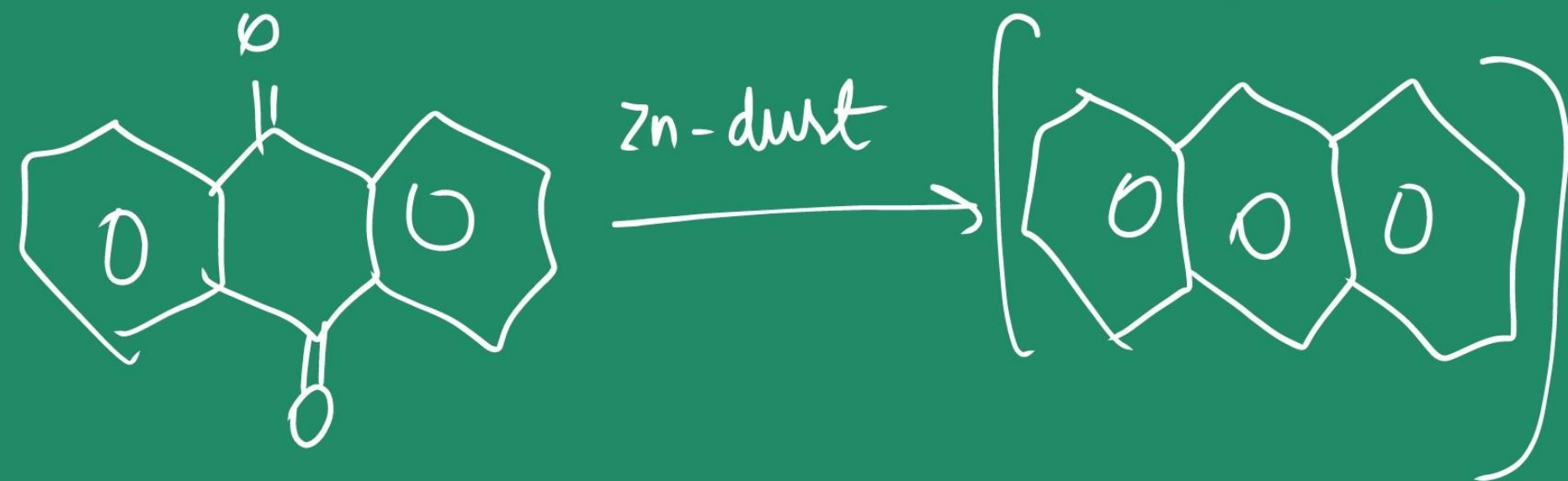
This reaction proceeds in many steps;



Now, Ring closure reaction takes place which proceeds to the closing of ring.



Now directly react with zinc dust for the formation of major product.



Physical

- It is a colourless solid.
- melting point: $\sim 218^{\circ}\text{C}$
- Boiling point: 340°C
- Insoluble in water but soluble in many organic solvents.

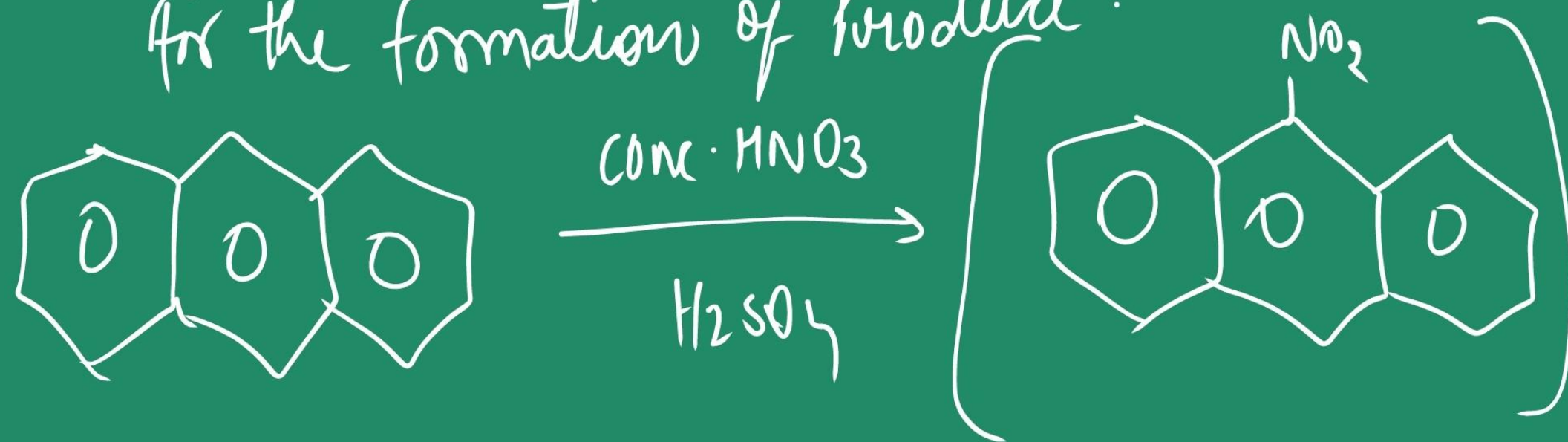
Chemical Properties

It also gives Electrophilic Substitution reaction.

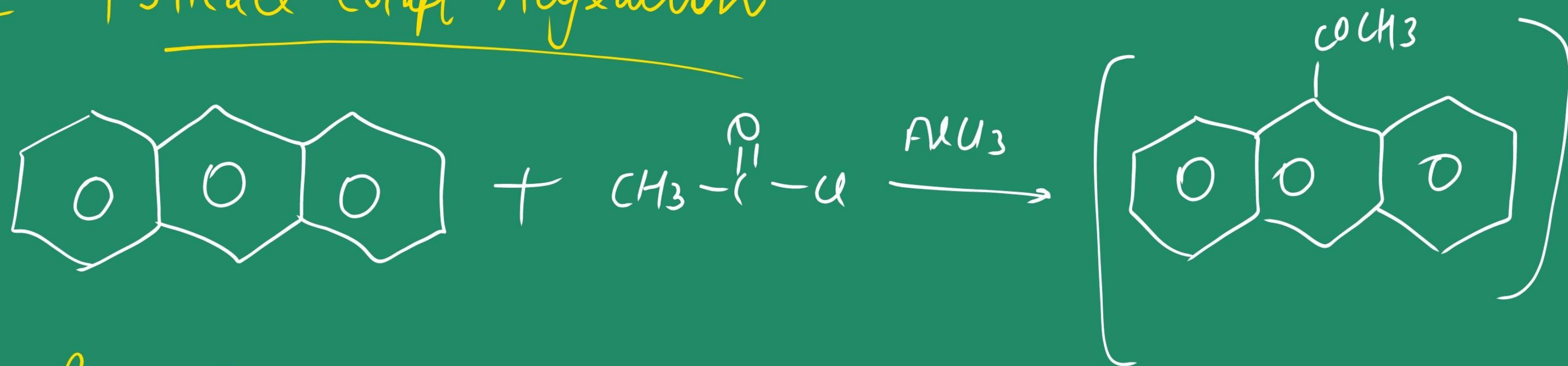
Preferentially occurs at C-9 and C-10 respectively.

1) Nitration

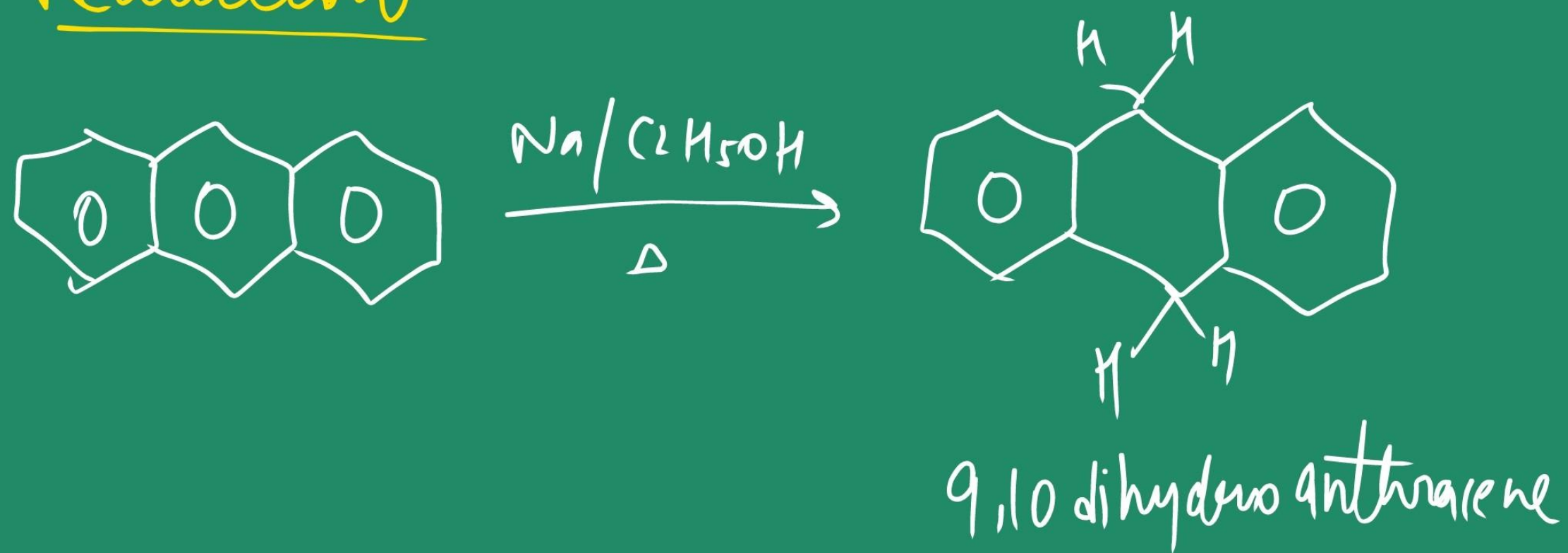
Anthracene reacts with conc. HNO_3 in the presence of H_2SO_4 for the formation of product.



2. Friedel Craft Acylation

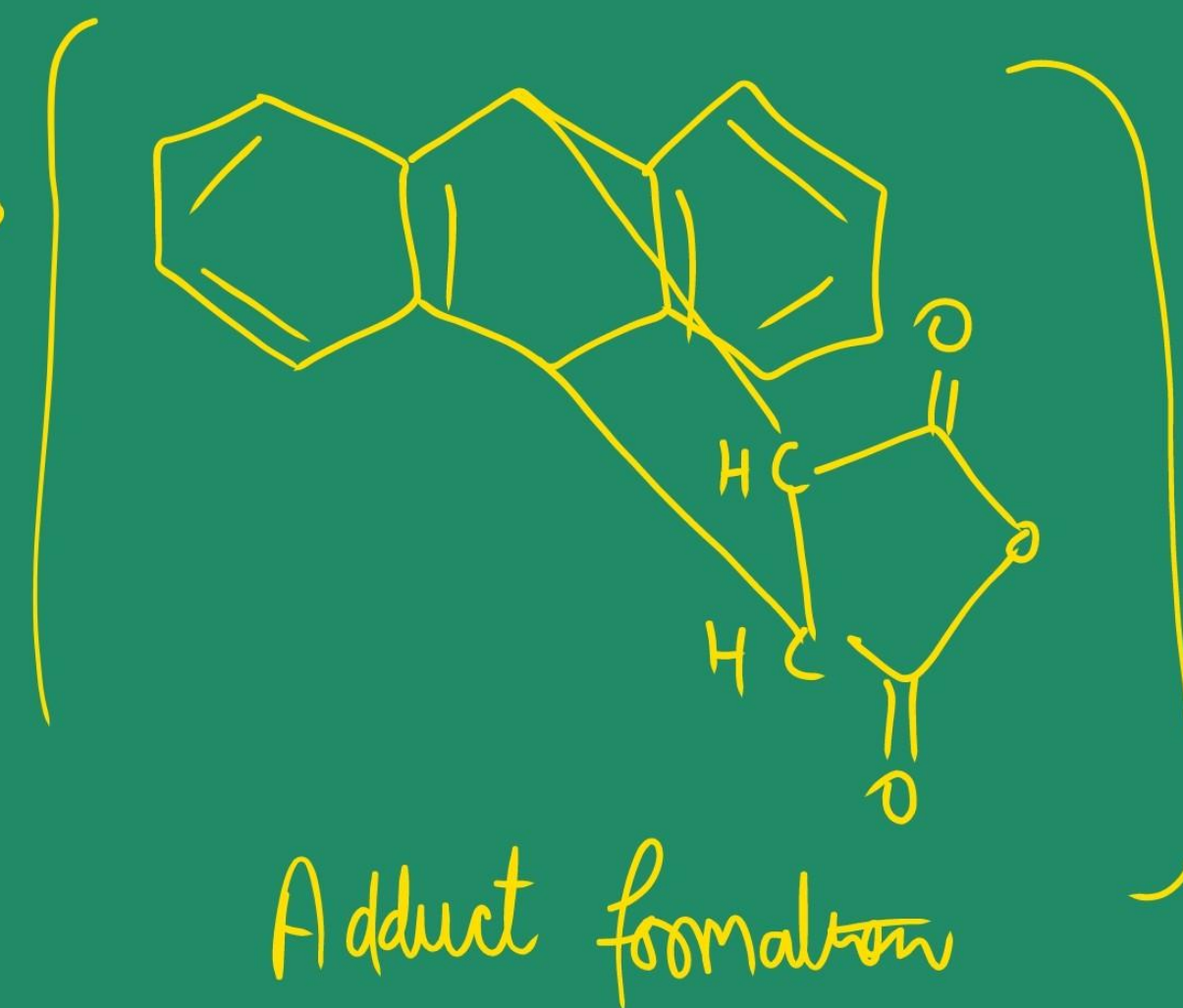
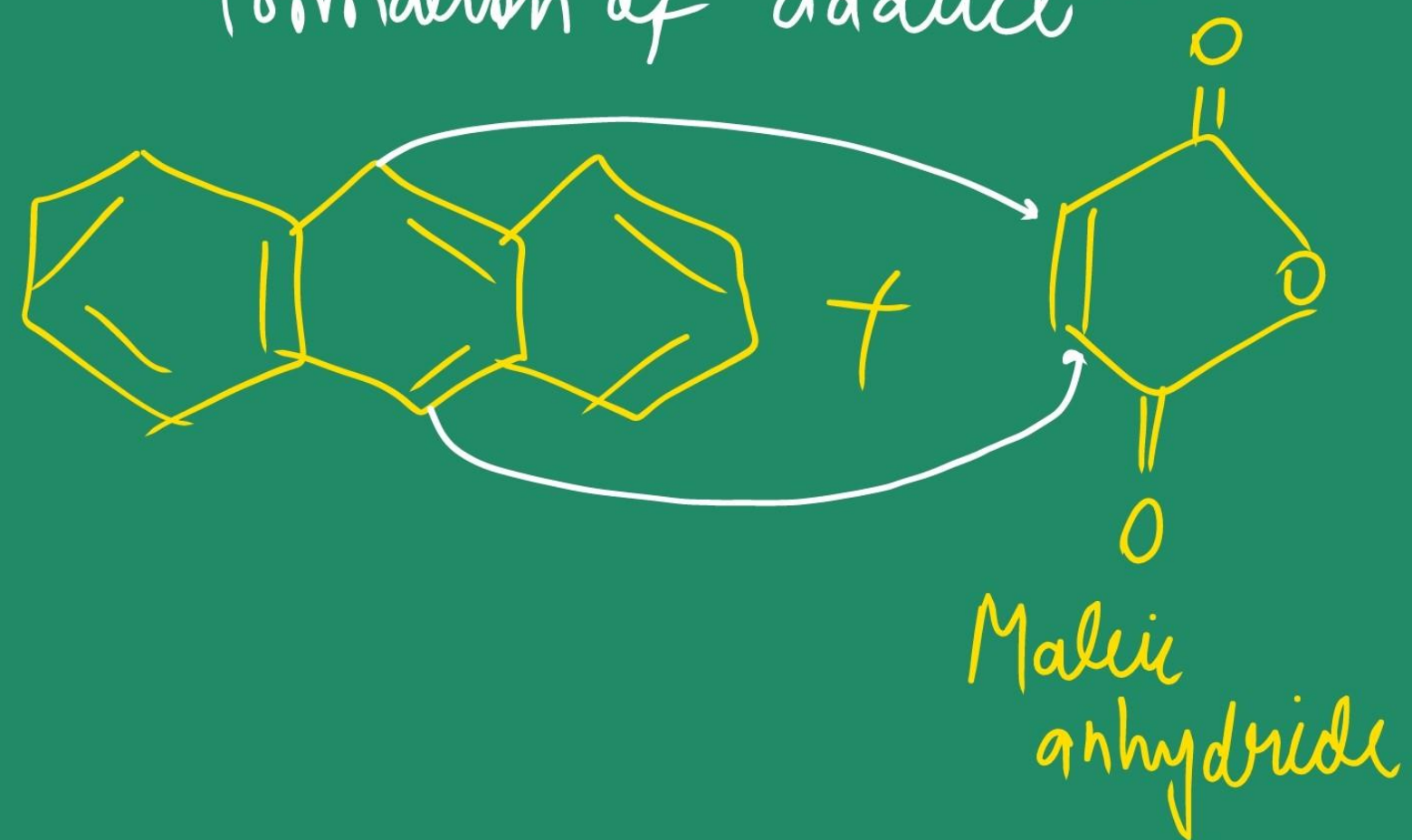


3. Reduction



Diels-Alder Reaction

Anthracene undergoes Diels Alder reaction for the formation of adduct



Medicinal Uses

- It is used as a preservative in wood.
- Used in the formation of many kind of dyes.
- Used in the formation of drugs.

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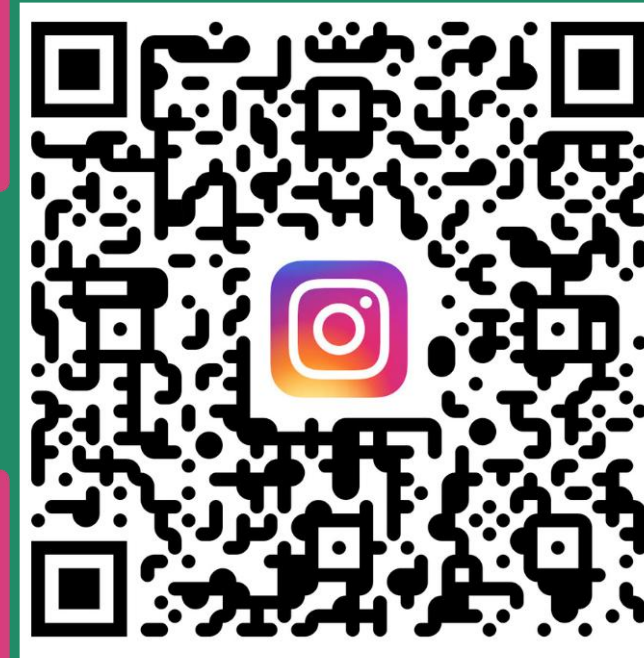
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POLYNUCLEAR HYDROCARBONS

DI - PHENYL METHANE

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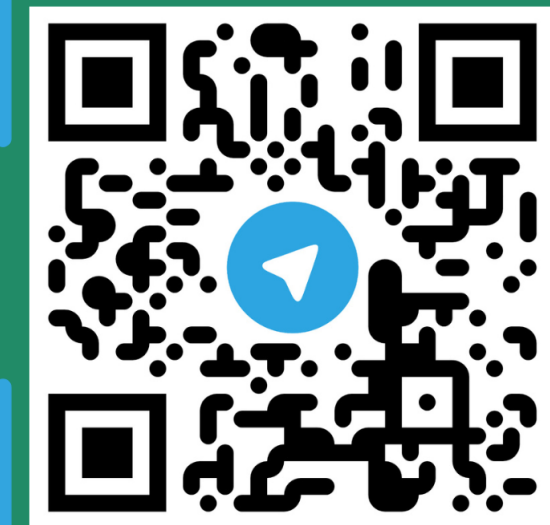
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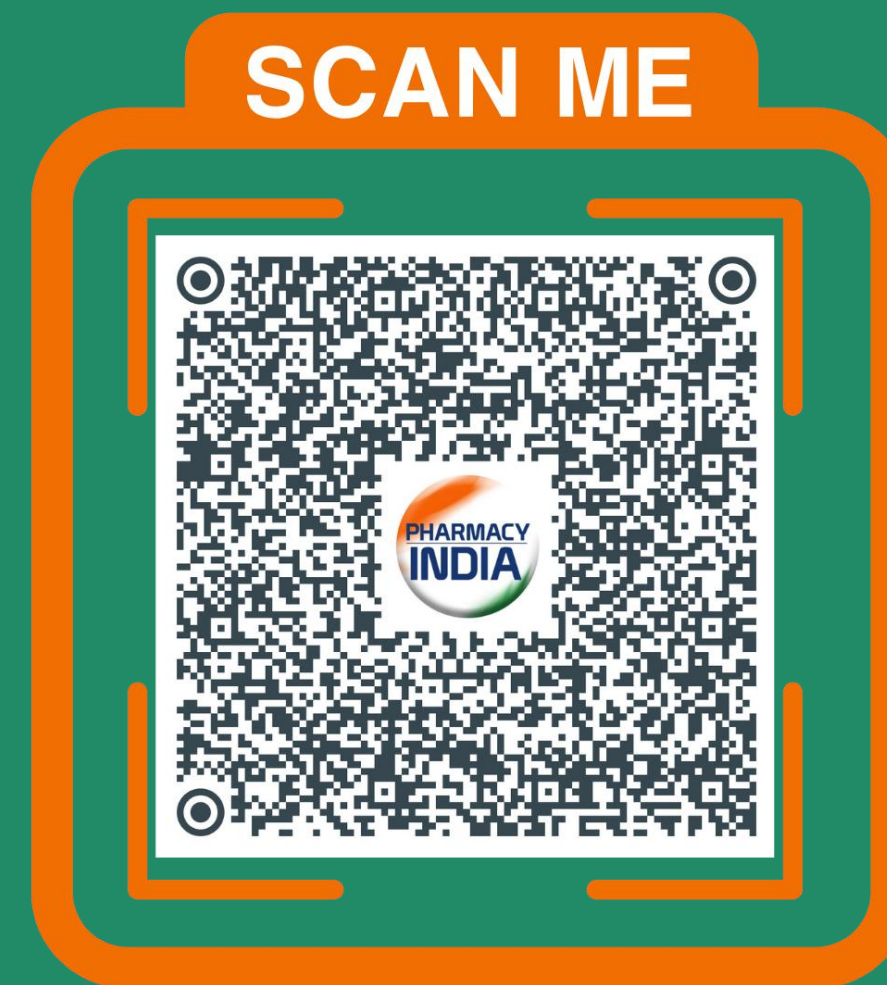


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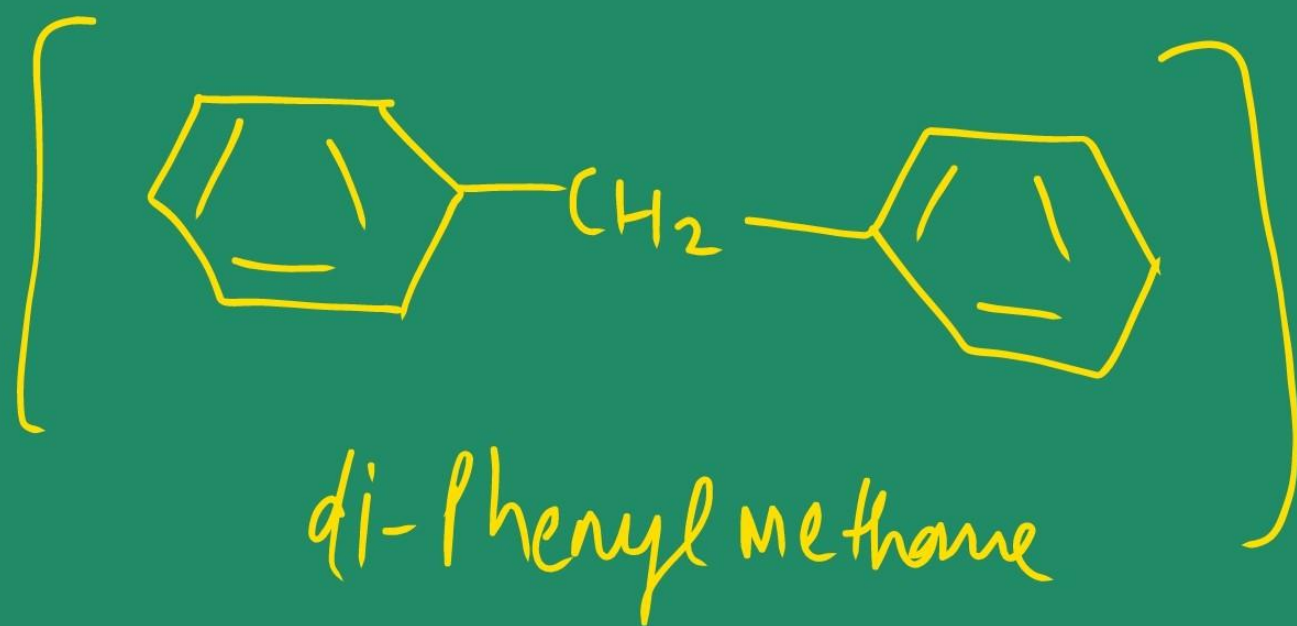
UNIT-4

TOPIC:- Di-Phenyl Methane

Di-Phenyl Methane

In this compound, two Phenyl rings are available along with one C-atom.

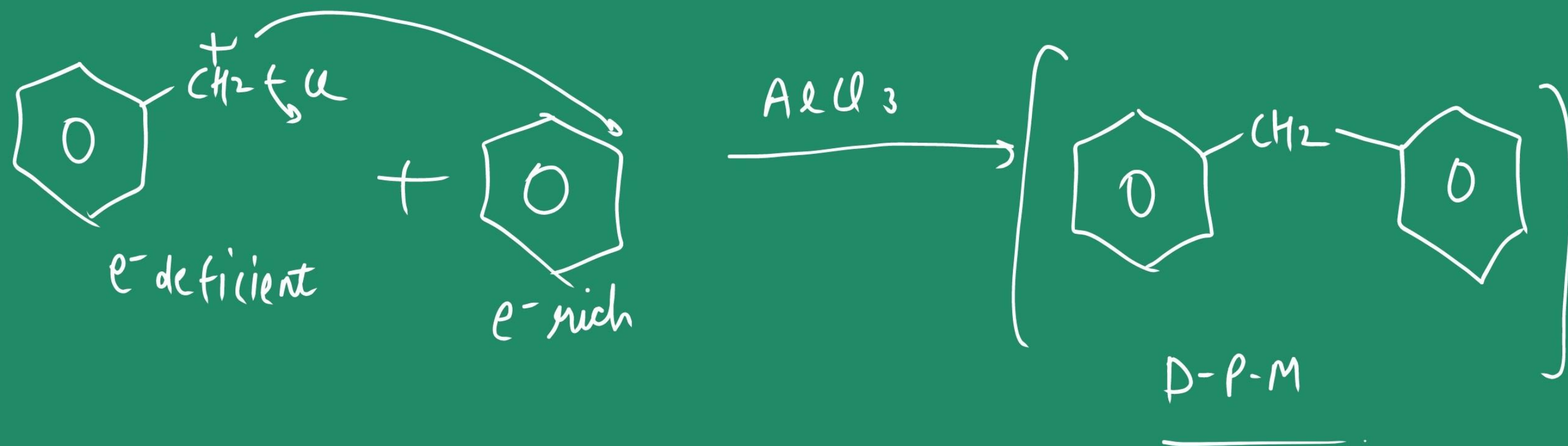
It's structure can be drawn as follows;



Synthesis

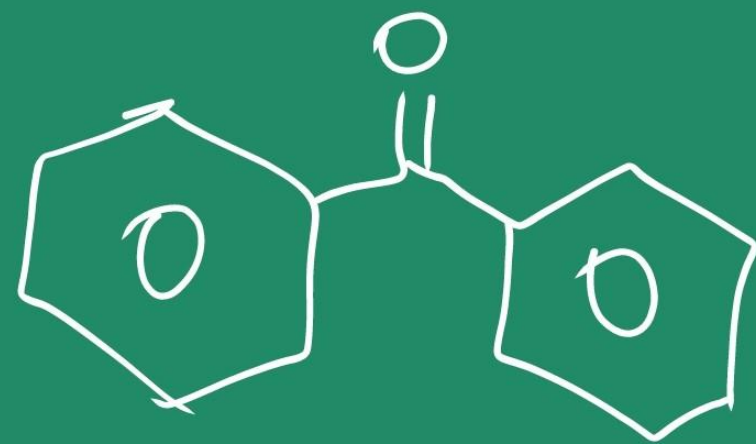
1. > Friedel Craft Reaction :- Di-Phenyl Methane can be Prepared by

Friedel Craft's condensation between Benzene & Benzyl Chloride.

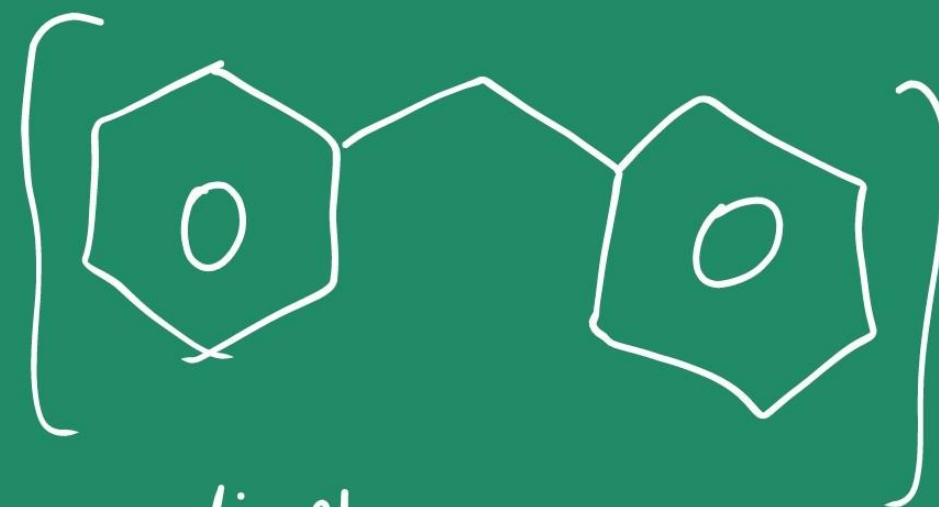


2. From Benzophenone

It is reduced in the presence of Red hot Phosphorous & HI.



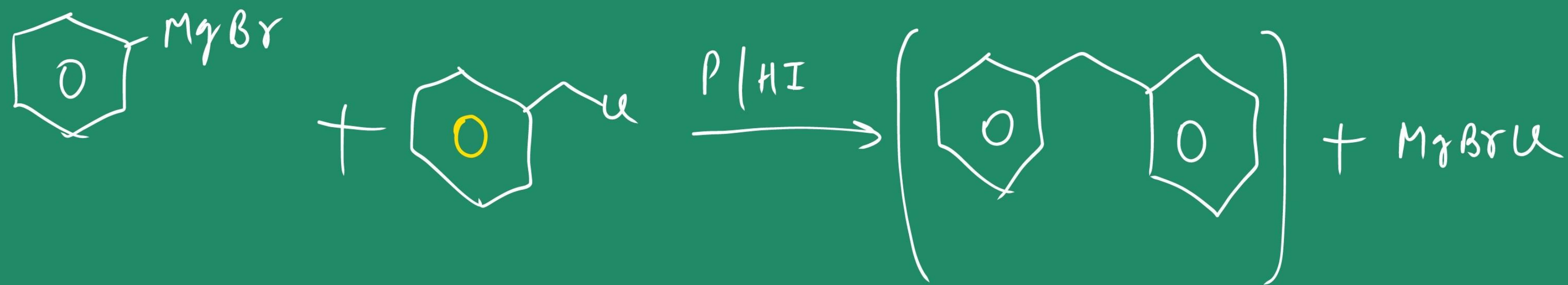
Benzophenone



di-Phenylmethane

3. From Grignard Reagent

Di-Phenyl Methyl can be easily Prepared by this method
using grignard reagent ($R\text{MgX}$).



Physical Properties

- Di-Phenyl methane is a colourless oil.
- Melting Point: $22 - 24^{\circ}\text{C}$
- Boiling Point: 264°C

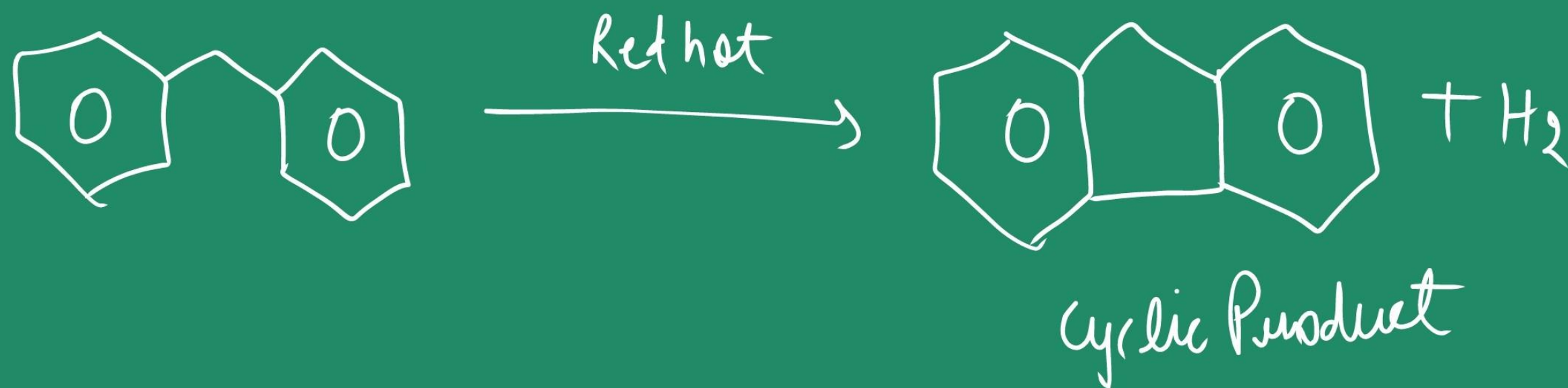
Chemical Properties

di-Phenyl Methane shows many type of Chemical reactions

Which are as follows;

1. Cyclization —

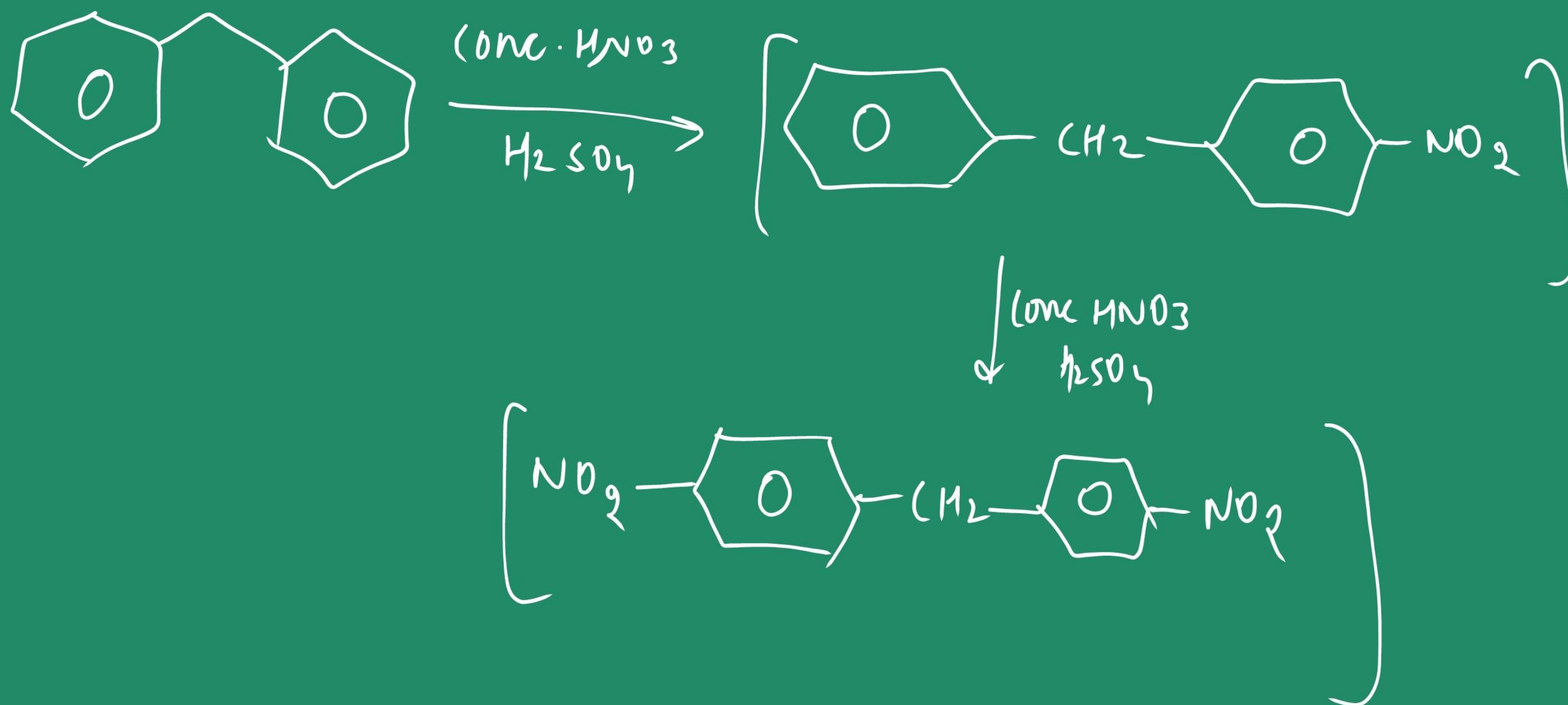
When di-Phenyl Methane is heated, a cyclic compound Produces.



2.

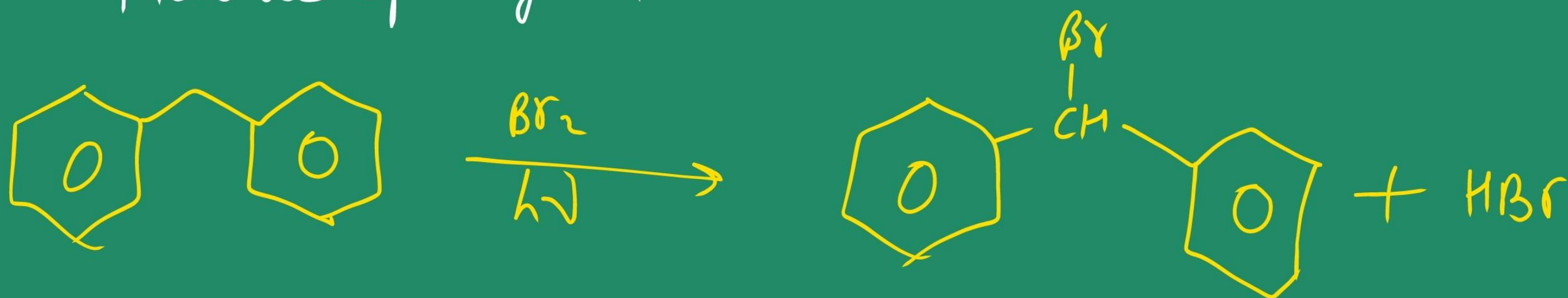
Nitration

In this reaction, di-Phenyl Methane reacts with conc. HNO_3 in the presence of H_2SO_4 .



3. Halogenation

In this reaction, di-Phenyl Methane reacts with halogen in the presence of light.



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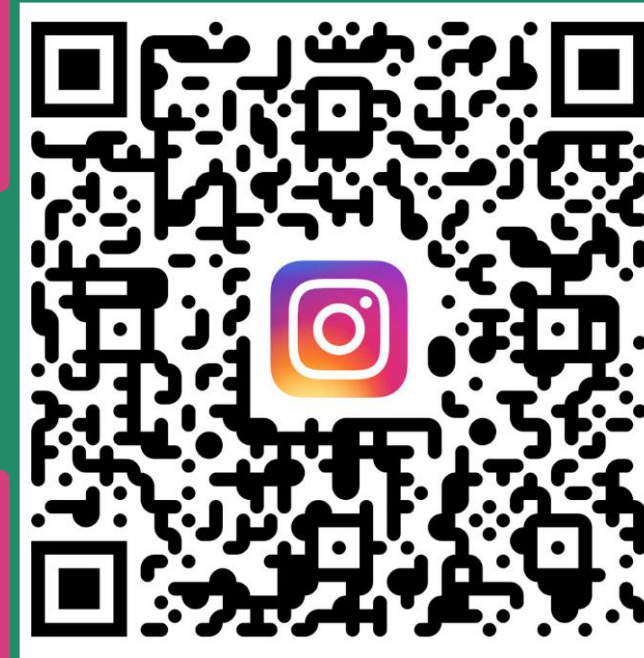
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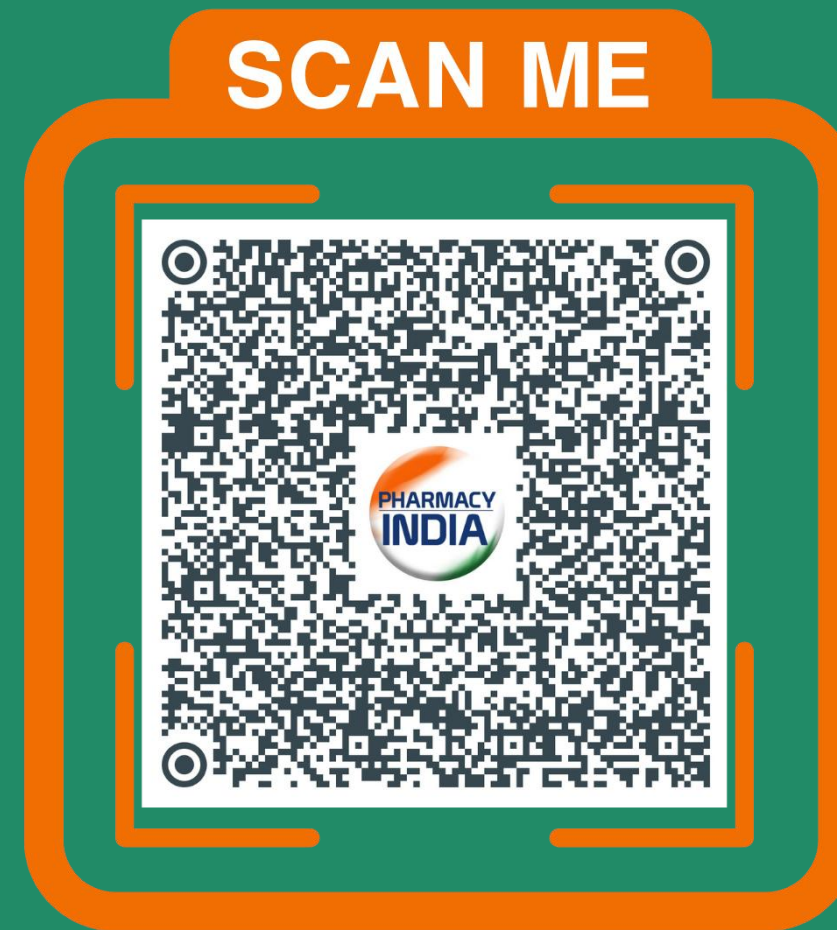
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POLYNUCLEAR HYDROCARBONS

TRI – PHENYL METHANE

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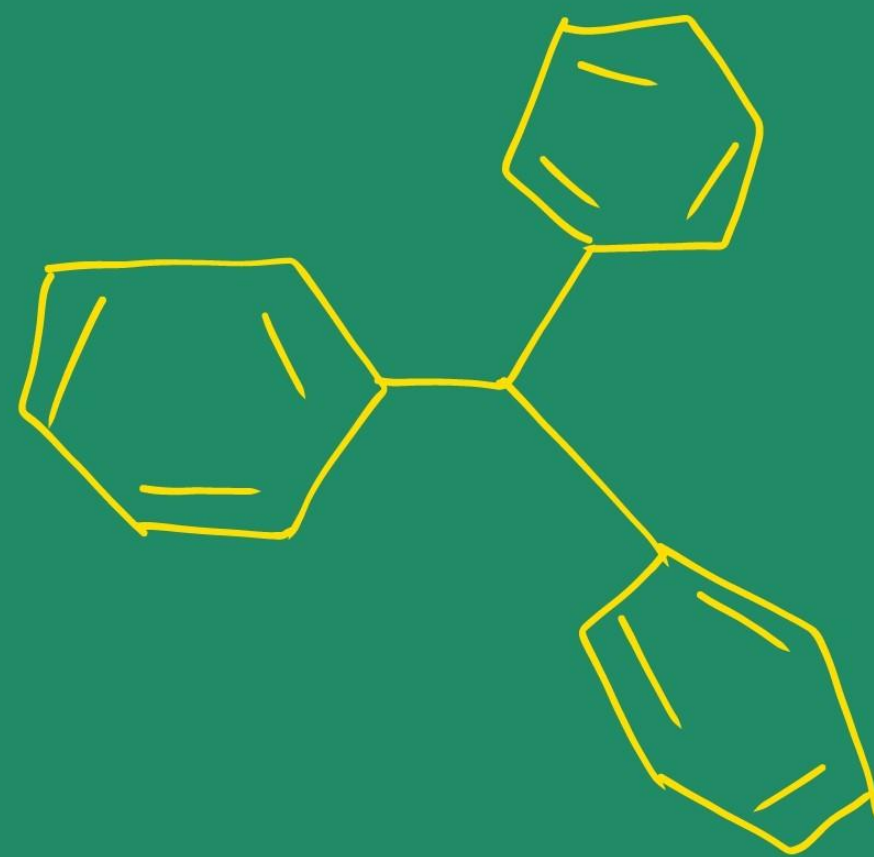
UNIT-4

TOPIC:- Triphenyl Methane

Tri- Phenyl Methane

It is a Poly-nuclear hydrocarbon which consists of three Phenyl rings.

Structure



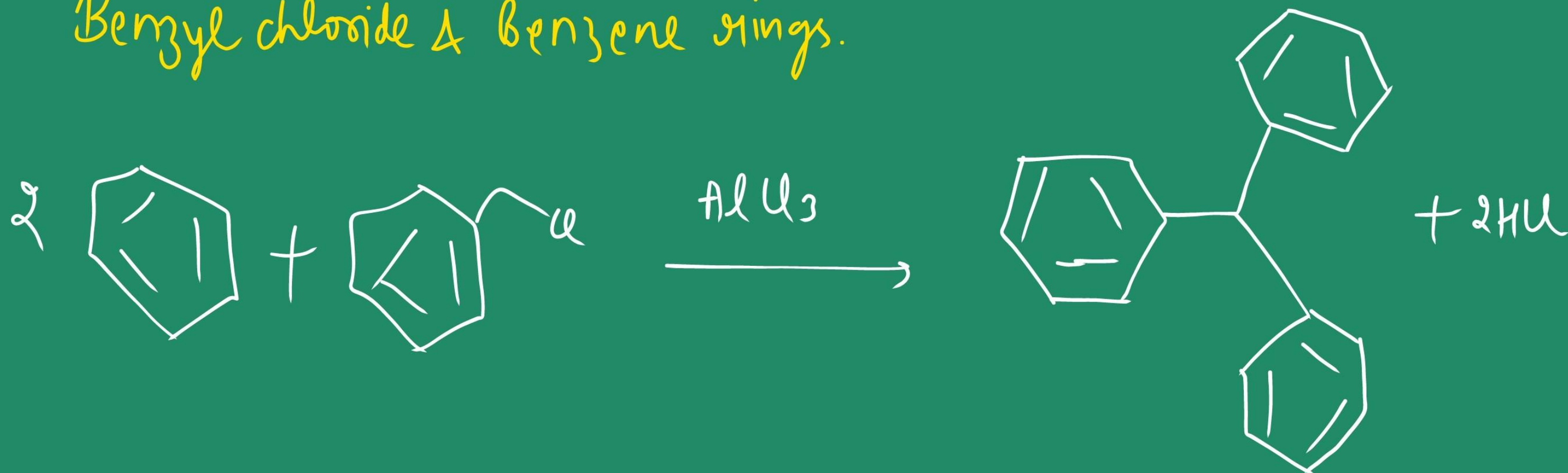
One C-atom is attached with three Phenyl rings.

→ Here C-atom is sp^2 -hybridised.

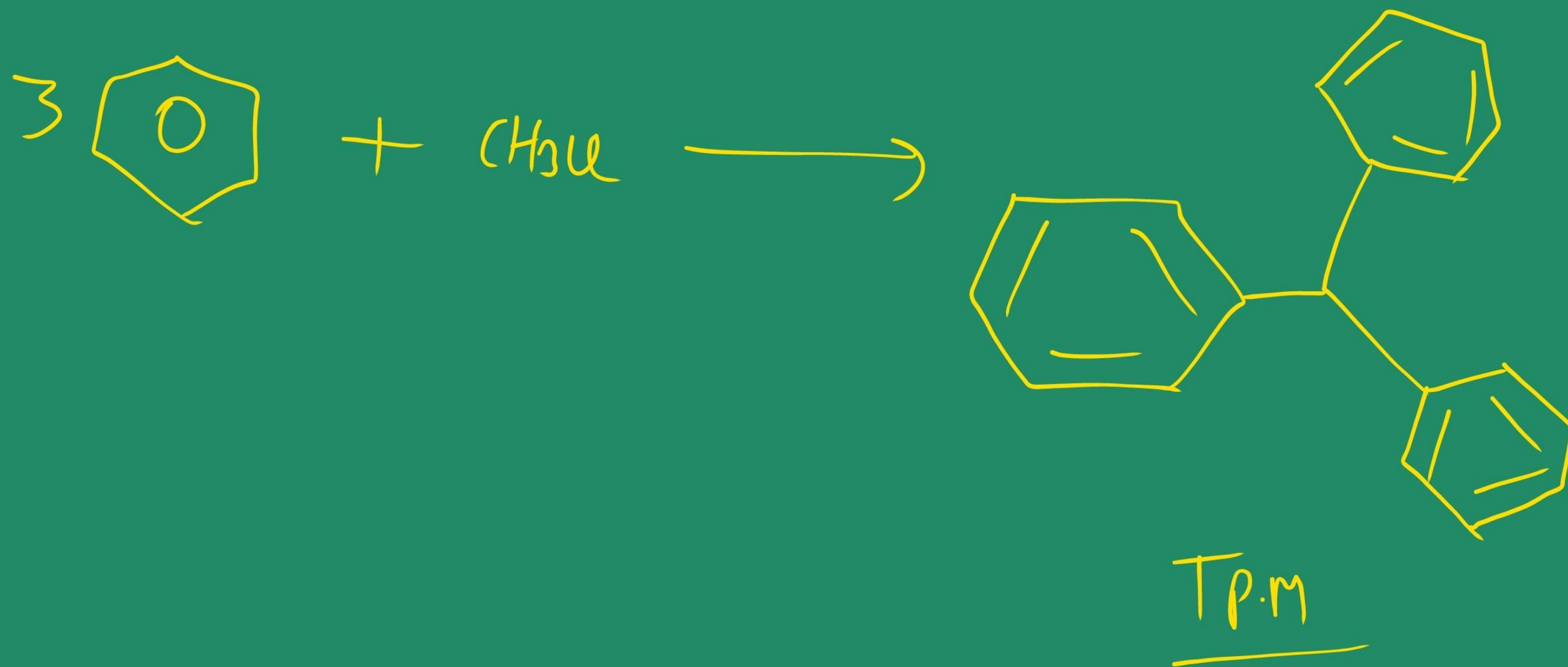
Methods of Preparation

1.7 Friedel - Craft reaction

Tri-Phenyl methane can be obtained after the condensation of Benzyl chloride & Benzene rings.



2. Benzene reacts with chloroform (CHCl_3) in the presence of any Lewis acid, formation of Triphenyl Methane takes place.



Physical Properties

→ It exists as a colourless solid.

→ Boiling Point : 359°C

→ Melting Point : $92-94^{\circ}\text{C}$

Medicinal Uses

1. It is a tri-aryl methane which is a backbone for the synthesis of dyes.
2. It has also been shown to inhibit 3-methyl chloro anthracene induced neo-Plastic transformation of lenti cells.

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