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CHM 405

Pharmaceutical Industry : They deal with pharmaceuticals

Pharmaceuticals

Active Pharmaceutical Ingredient

(1) Drug molecules (API)

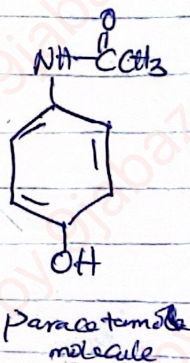
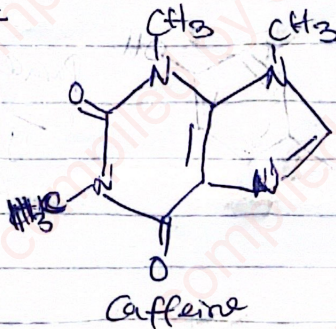
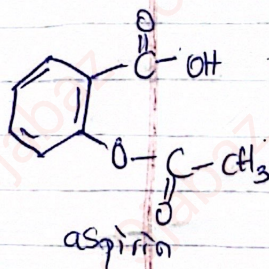
(2) Excipients : The most important excipient for tablet is Starch.

The starch functions as a binder for the drug molecule, it make the drug hard.

Anything to be used in the pharmaceutical industry must be 99.9% Pure, very pure.

The starch used in the pharmaceutical industry is Corn Starch

API



amin C - Ascorbic acid

polypropylene is resistant to chemical attacks.

Solutions (intravenous)
(1) Saline, ionic
(2) Therapeutics

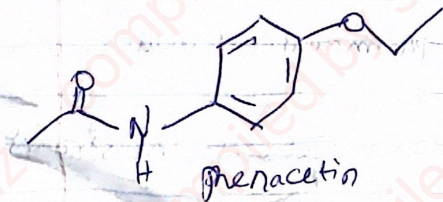
fat soluble

- (4) Injection (5) Emulsion (6) Stabilizers e.g. Tocopherol, ascorbic acid
(7) Vaccines (8) Antibiotics

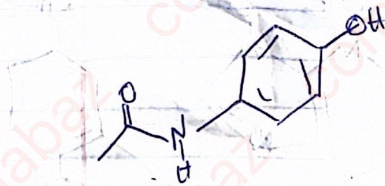
water soluble

Assignment

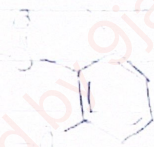
Get more list of Pharmaceuticals.



Phenacetin



Paracetamol
Tylenol

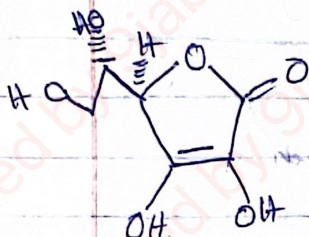


Tocopherol structure

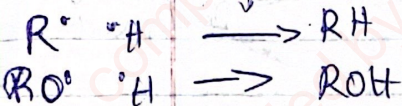


It can behave like an antioxidant

oxidant helps to preserve the shelf life of a molecule



ascorbic acid



Chemist do;

- (i) organic synthesis
- (ii) process chemistry
- (iii) Chemical eng
- (iv) Industrial chemistry

Difference between API vs Tablet

-g Paracetamol API is the drug molecule
 paracetamol tablet is the drug molecule + excipients
 + stabilizers

Chemistry do

Analysis (i) Purity level (ii) Quality control

API

- ① Non Steroidal Anti inflammatory agents (NSAIDs)
- ② Antimicrobial agents
- ③ Antimalarials
- ④ Anti depressants

* Research & Development (R&D) † Drug Design and Development

100 Organic Synthesis

20% Pharmacology

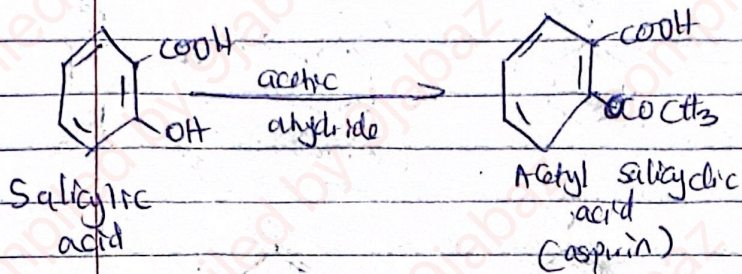
10% Biochemistry

10% Microbiology

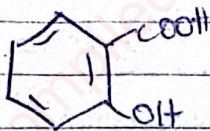
NSAIDs

- (i) Aspirin
- (ii) Paracetamol
- (iii) Ibuprofen
- (iv) Naproxen
- (v) Diclofenac
- (vi) Indomethacin

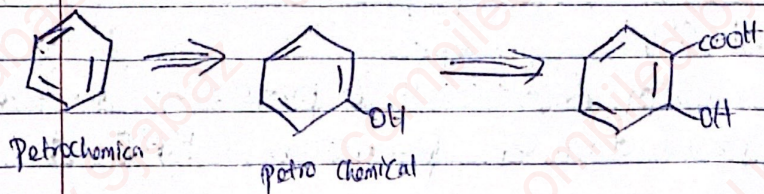
Aspirin Preparation



Starting Material



① salicylic acid. What is the source??



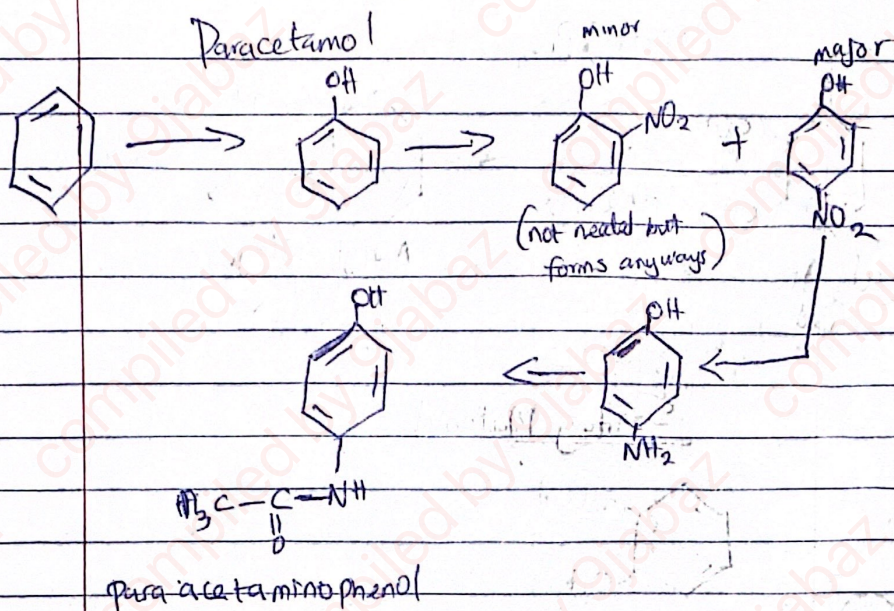
② Determine if it will be economical to produce natural or synthetic means

③ salicylic acid through petrochemical

① Condition

② Chemical reaction

④ Equipment

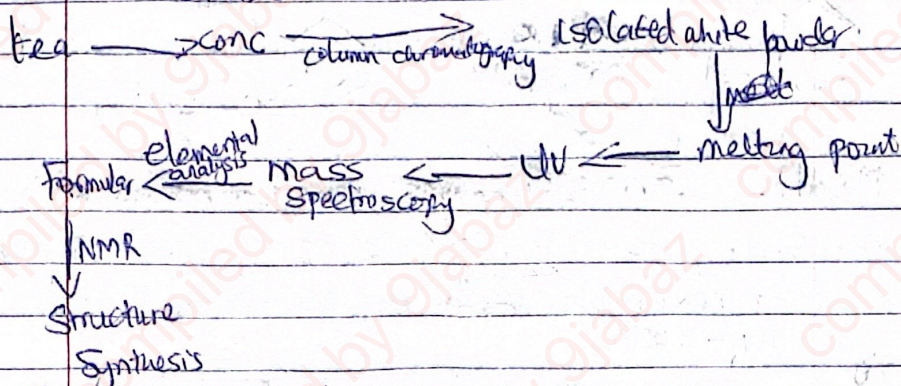


What is the industrial production of paracetamol, write all steps.

- ① In the industry, describe all the process and conditions for the production of paracetamol API

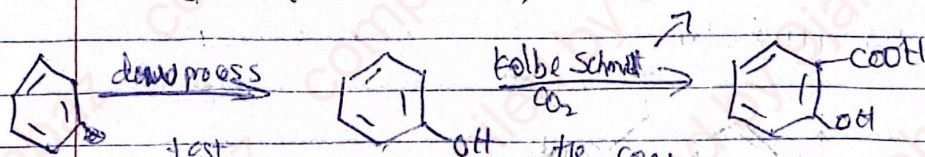
Down process

13/11/2025



The pharmaceutical company is a petrol halide industry.

Salicylic acid can be ~~start~~ gotten starting with benzene (from petrochemicals) conditions; H_2SO_4 catalyst



Explain down process and ~~how~~ to get conditions to get a good yield.

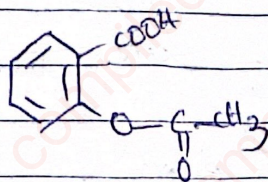
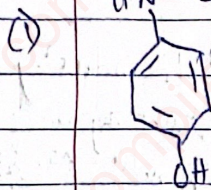
Condition

- (i) catalyst
- (ii) temperature
- (iii) pressure
- (iv) solvent

If the temperature is $105^\circ - 150^\circ C$ it favours the ortho product but if the temperature is $220^\circ - 250^\circ C$ it produces the para product. Side Effect started showing up e.g. ulcer due to the phenolic OH, then it was mitigated by acetylation.

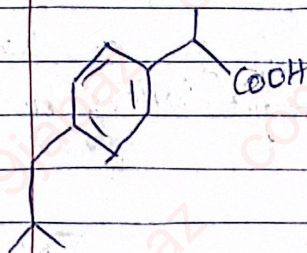
CC1(C)C(C)C(C)C(C)C1C(=O)O

~~acidification~~
anhydride


$$H\ddot{N}-COCH_3$$


It has been made to have the therapeutic feature of Salicylic acid and not cause ulcer, which has been successful.

(11) Thick of an



Pre-cursor molecule is the one that we can do a slight modification to get our target molecule.

Precursor

Target molecule

breakdown in biological system
metabolite

Industrial Processes for making API

- (1) The reaction(s): Feasibility is considered
- (2) Reagents: Source, affordability is considered
- (3) Condition: affordability, infrastructure is considered.

Assignment & test

Kinds of reactors in industry.

(4) Work-up

- (i) filtration
- (ii) recrystallization
- (iii) Purification (Chromatography)
- (iv) Analysis

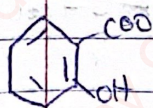
test.
Find out what type of chromatography

test
What are the considerations

What do you consider in analysis??

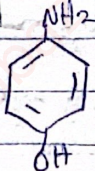
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Aspirin



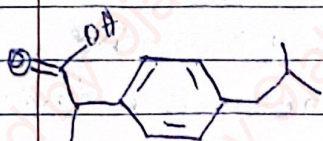
precursor molecule

Paracetamol



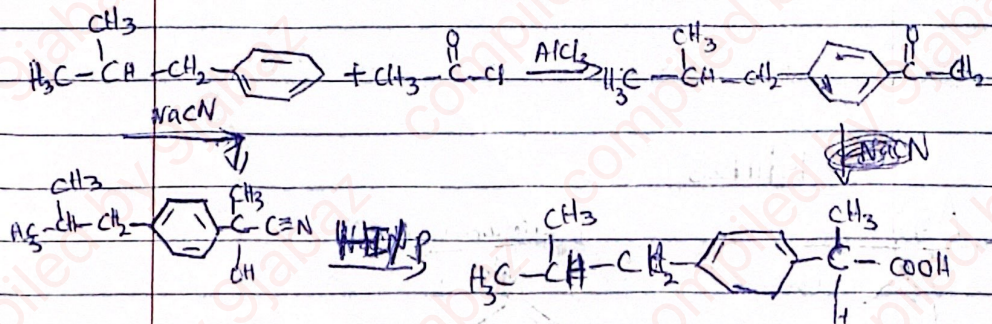
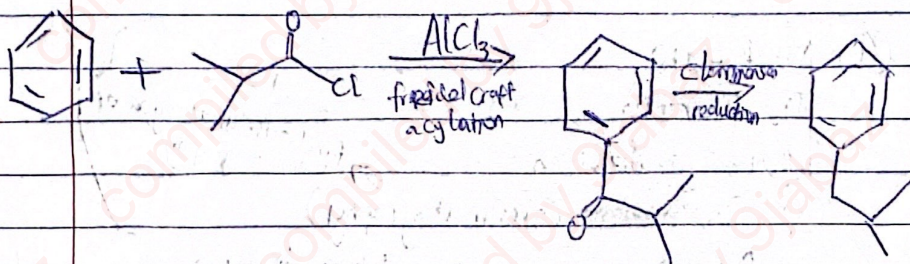
precursor molecule

Ibu profen



Ibuprofen

We can start with benzene



* Why Grignard reagent not used?

Atom economy is a measure of the efficiency of a chemical reaction, specifically the proportion of reactant atoms that are incorporated into the desired products.

Boots synthesis sep; it is 40% atom efficient

- (1) Friedel acylation of isobutyl benzene with acetyl chloride
- (2) Darzens reaction with ethyl chloroacetate to form epoxy ester
- (3) Hydrolysis and decarboxylation to form an aldehyde
- (4) Condensation with glyoxyamine to form an aldoxime
- (5) Dehydration of the aldoxime using acetic anhydride to yield the nitrile
- (6) Acid-catalyzed hydrolysis of the nitrile to the final carboxylic acid (ibuprofen)

White is not a colour, all colours originate from white

Dr. Tarek's Post

CHM 405

- ① Dyes and pigments
- ② Steel Industry
- ③ Soap and detergents
- ④ Textiles

Chemistry of Dyes and Pigments

Dyes and pigments are important classes of coloured compounds used extensively in textiles, paper, in food, plastics, cosmetics, and art industry, also in automobiles.

Both dyes and pigments are substances that impart colour, but they differ mainly in their solubility and the way they interact with the substrate.

Differences Between Dyes and Pigment

Feature	Dye	Pigment
① Solubility	Dyes are soluble in water or suitable solvent (water soluble)	They are insoluble in water or organic solvents (water-insoluble). They are soluble in inorganic solvents.
Application	Dyes penetrate and chemically bond with fibers.	The adher or stick to surface with dispersion or binder.

* Low ΔG , high electrophilicity difference
* Low ΔG , low electrophilicity difference

(small atoms)
(high electrophilicity)

Feature	Dyes	Pigment
(3) Bonding Mechanism	Chemical affinity between the dyes and the substrate (Ionic, Covalent, hydrogen bonding; van der Waals).	It is purely physical adsorption.
(4) Examples	Methylene Blue, Congo Red, Alizarine, Methyl orange	Titanium dioxide, Prussian blue

Origin and Historical Background

The use of dyes and pigments dates back thousands of years. Natural dyes are derived from plants, animals and minerals.

Examples

- (1) Indigo is obtained from Indigofera tinctoria (blue dye)
- (2) Alizarine from Madder root. Rubia tinctorum,
- (3) Cochineal from carminic acid extracted from insect
- (4) Tyrian Purple obtained from mollusc (most expensive)
6, 6'-dibromoindigo

Synthetic Dye

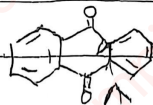
Synthetic dye began with William Henry Perkin's accidental discovery of mauveine in 1856 from Aniline. This discovery marked the ^{birth} of the synthetic dye industry.

Azo dyes are nitrogen containing dyes
 & structure

and modern organic chemistry

Classification of Dyes

Dyes can be classified by chemical structure or by their application



Class of dyes	Example	Functional groups / Chromophore
Azo dye	Methyl orange, Congo red	
1) Azo dye	Methyl orange, Congo red	$-N=N-$
2) Anthraquinone dyes	Alizarin	Anthraquinone nucleus
3) Triphenylmethane dyes	Crystal violet	The central carbon linked to three phenyl ring
4) Nitro and Nitroso dyes	Preric acid Preric acid	$-NO_2, -NO$
5) Phthalocyanine dye	Phthalocyanine blue	A large macrocyclic system with metal ion

Classification by Application

- (1) Acid dyes: ^{used} for woods, silk. Example of such as orange II
- (2) Basic dyes: used to dye acrylic materials. Example is methylene blue
- (3) Direct dyes: Applied directly to cotton. Example, Congo red
- (4) Vat dyes: These are insoluble dyes reduced to soluble form ^(application) during dye. ~~Vat dye~~ Example is indigo
- (5) Dispersed dyes: These are used for hydrophobic fibres

Chemical properties of Dyes and Pigments

- (1) Chromophore: Bunch of functional groups that gives colours to substances. The colour of the dye is due to certain groups ^(functional groups) containing multiple bonds known as chromophores.

Examples: NO_2 , NO , $-\text{CO}-$, $-\text{C}=\text{C}-$, $-\text{C}\equiv\text{C}-$, C
nitro, nitroso, carbonyl

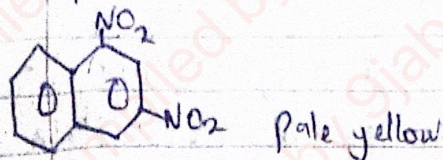
As the number of chromophore increases for a dye, the colour of the dye ~~also decreases~~ deepens.

- (2) Auxochromes: They are not chromophores in the sense that they don't give colour, but their presence increases the intensity of the colour, it deepens the dye. They are groups that modify the solubility and the intensity of the colour.

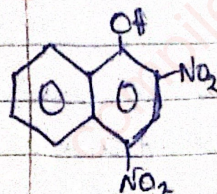
27) Auxochromes:

examples, $-OH$, NH_2 , NHR , NR , (Cl, Br, I) , $-SO_3H$,
 $-COOH$

for example, 1, 3, dinitronaphthalene



But when Auxochrome is present, e.g. OH



(2, 4, dinitrophenol)

yellow $\rightarrow$ orange red.

The colour becomes, orange red.

Resonance and Conjugation

Extended π -conjugation lowers the energy gap between the HOMO and LUMO. This results in the shifting of absorption into the visible region.

Acid-Base properties

pH can change dye colour due to structural resonance
e.g. phenolphthalein

Valence is the number of bond surrounding an atom
+ valency is the combining power

Valence Bond theory

In the ground state, the electron pair of a molecule are in a state of oscillation, not vibration and absorb a photon of appropriate energy and gets excited when placed in the path of a beam of light.

The wavelength of the photon of light absorbs depends upon the energy difference between the ground state and the excited state.

Molecular Orbital theory

According to molecular orbital theory, whenever a molecule absorbs a photon of light, ~~one~~ electron is transferred from bonding (non-bonding orbital) to an antibonding molecular orbital. Based on different type of electrons present in a molecule, different types of electron transition are possible.

Synthesis of Dyes

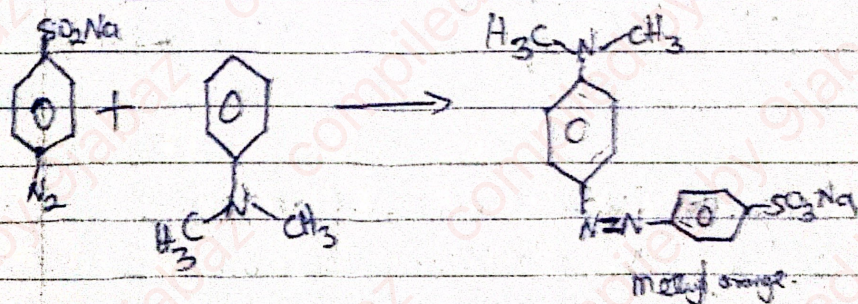
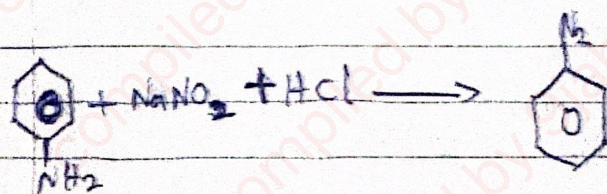
- (1) Azo dyes: These dyes constitute the largest part of the synthetic dyes. The chromophore of the Azo dye is an aromatic system joined with the azo group and the ~~single~~ of an auxochrome.

Ar dyes are classified according to the number of azo groups in the molecule. We can have a mono azo dyes, di azo dyes, tri azo dyes.

1st step: Examples: Methyl orange, an example of mono azo dyes.

Methyl orange is synthesised / obtained by converting aniline into a diazonium salt (diazotization)

2nd step: Coupling reaction. The diazonium salt reacts with another aniline in an alkaline medium



Properties of Methyl Orange

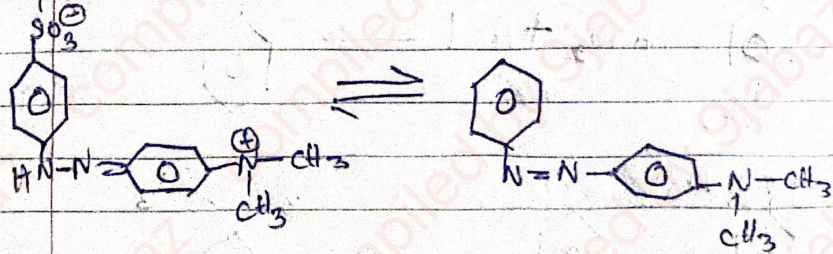
Methyl orange is a colouring dye for wool and silk, but its colour fades on the exposure to light and washing, usually it is not used as dye, but used as an indicator in the

acid base titration

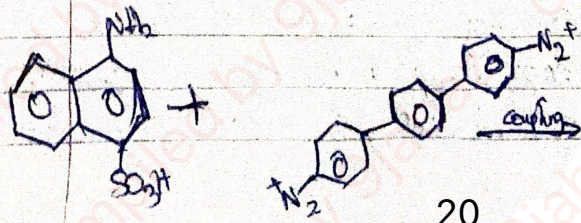
The ~~ph~~ pH range of methyl orange is between 3.1-4.4. It is yellow in basic solution and red in acidic solution.

The colour change takes place because of the change in the colour of ions ⁱⁿ ~~because~~ of basic and acid medium. In acidic medium, the ion contains p-quinone, while in basic medium it contains azo

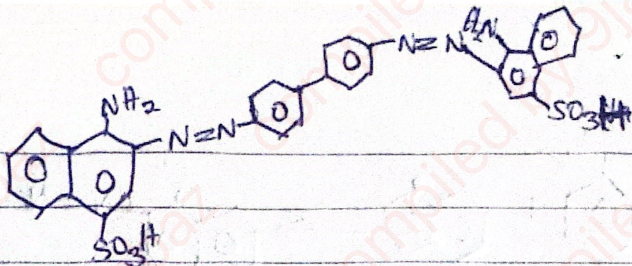
chromophore



Comp red: It is an example of diazo dye. It contains two azo groups. It is prepared by coupling of tetraazotized Persidine with two molecules ~~not~~ naphthionic acid (4-aminonaphthalene-1-sulfonic acid)



Coupling →



It is a direct dye and sodium salt of this dye gives red colour on the application to cotton.

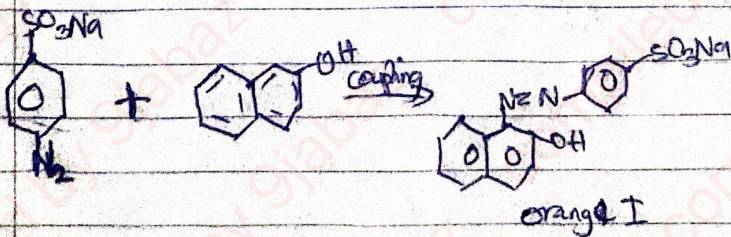
On addition of acid, its colour changes, because of this, it is not used as dye generally, mostly, it is used as an indicator.

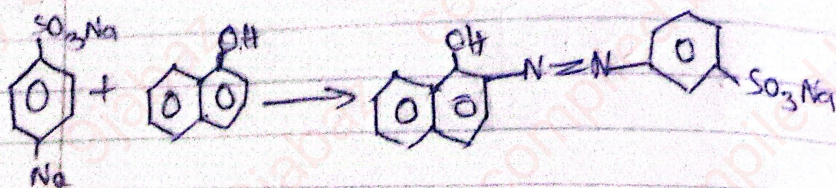
It is blue in acidic solution and red in solution above pH of 3.

The change in colour from red to blue in acidic solution is due to the resonance among the charged canonical structure.

Orange I:

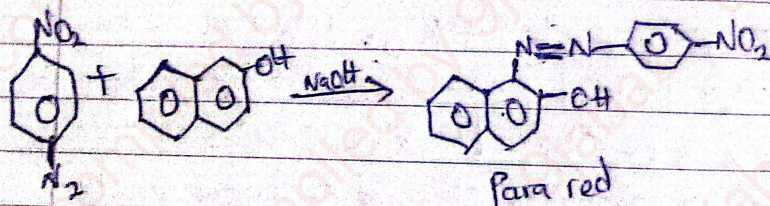
Orange I and Orange II which are examples of acid dyes can be obtained by coupling diazotized sulphonic acid with α - and β -naphthol.





Para Red

Para red are used in foodstuffs, cosmetics, drugs and as an indicator



1-(4-nitrophenyl) diazenyl
naphthalene-2-ol