JHARKHAND
Rai University
UGC RECOGNISED UNIVERSITY
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PRACTICAL LAB MANUAL

Medicinal Chemistry - III

B. Pharm VIth Semester

CONTENT

Experiment No: 01

Synthesis of Sulphanilamide

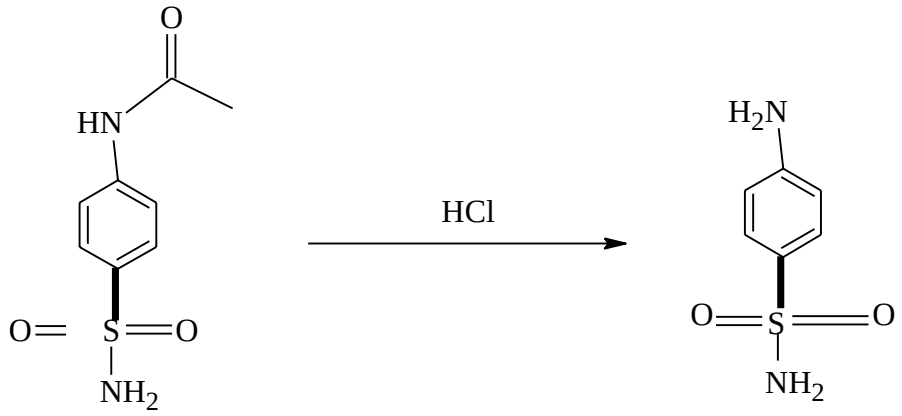
Aim:

To synthesis and submit sulphanilamide from p-acetamido benzenesulphanilamide and calculate its percentage yield.

Principle:

Sulphanilamide can be prepared by the reaction of P-acetamido benzene sulphanilamide with Hydrochloric acid or ammonium carbonate. The acetamidogroups are easily undergo acid catalysed hydrolysis reaction to form p-amino benzene sulphonamide.

Reaction:



4 Acetamidobenzene sulphonamide p Amino benzene sulphonamide

Chemical Required:

Resorcinol - 1.2 g

Ethyl acetoacetate - 2.4 ml

Conc. Sulphuric acid - 7.5 ml

Procedure:

1.5 gm of 4- acetamido benzene sulphonamide is treated with a mixture of 1 ml of conc. Sulphuric acid diluted with 2 ml water. This mixture is gently heated under reflux for 1 hour. Then 3ml of water is added and the solution is boiled again, with the addition of a small quantity of activated charcoal. The solution is filtered while hot, and the filtrate is neutralised with powdered sodium carbonate with stirring until all effervescence ceases and the sulphanilamide is precipitated as a white powder. The solution is cooled,

filtered, the sulphanilamide wash with water and dried. Finally, crude sulphanilamide is recrystallized from hot water, to get colourless crystals.

Melting Point: 163^0C

Category: Bacteriostatic agent

Report:

The Sulphanilamide was synthesised and submitted, Reported the following

1. Theoretical Yield =
2. Practical Yield =
3. Percentage Yield =

Experiment No: 02

Synthesis of 7- Hydroxy -4- Methyl Coumarin

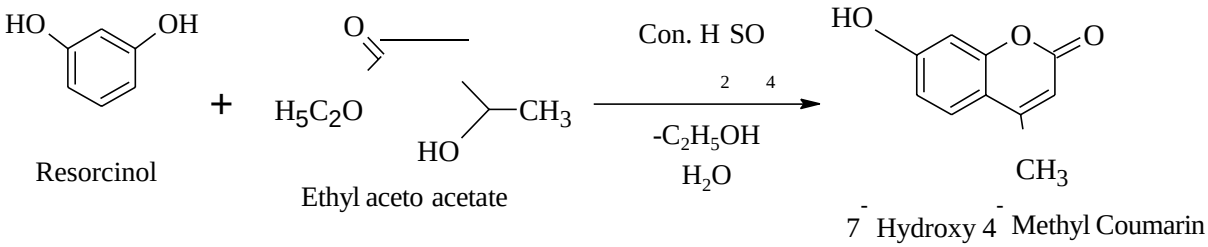
Aim:

To Synthesis and submit Synthesis of 7- Hydroxy -4- methyl coumarin**.**

Principle:

A general synthesis of coumarins involves the interaction of a phenol with a β- ketoester in presence of an acid condensing agent (Pechmann reaction). Concentrated sulphuric acid is usually used as the condensing agent for simple monohydric phenols and β- ketoesters, although phenol itself reacts better in the presence of aluminium chloride. The mechanism of the reaction to involve the initial formation of a β- hydroxy ester, which then cyclise and dehydrates to yield the coumarin. Polyhydric phenols, particularly here the two hydroxy groups are meta oriented, react with great ease and sulphuric acid is used as the condensing agent with careful temperature control to ensure a good yield.

Reaction



Resorcinol

Ethyl aceto acetate

7- Hydroxy 4- Methyl Coumarin

Chemicals Requirements:

Conc. Sulphuric acid-7.5 ml	Ice – q.s
Resorcinol – 1.2 g	Sodium Hydroxide- q.s
Ethylacetoacetate – 2.4 ml	Ethanol – q.s

Procedure

Take 1 litre of concentrated sulphuric acid in a 3 litres capasity 3 necked flask fitted with a thermometer, mechanical stirrer and a dropping funnel. Immerse the flask in an ice bath. When the temperature falls below 10^0C, add a solution of 100 g (0.91 mol) of resocinol in 134 g (130.5 ml, 1.03 mol) of redistilled ethyl acetoacetate drop wise and with stirring. Maintain the temperature below 10^0C by means of an ice-bath during the addition (2h). Keep the mixture at room temperature for 18 hr and then pour it into a mixture of 2 kgof crushed ice with vigours stirring and add 3 litter of water. Collect the

precipitate by suction filteration and wash it with three 25 ml portion of cold water. Dissolve the solid in 1500 ml of 5 percent sodium hydroxide solution, filter and add dilute 2 M sulphuric acid (about 550 ml) with vigourous stirring until the solution is acid to litmus. Filter the crude 4-methyl-7-hydroxy coumarin at the pump, wash with four 25 ml portions of cold water and dry at 100^0C. The yield is 155g (97%). Recrystallise from 95 percent ethanol: the pure compound separete in colourless needles, m.p. 185^0C.

Use

Laser dye.

Starting material for production of the insecticide ‘ hymecromone’.

Report:

7- hydroxy -4- methyl coumarin was synthesized and the percentage yieldwas found to be..... %.

Experiment No: 03

Synthesis of Chlorbutanol

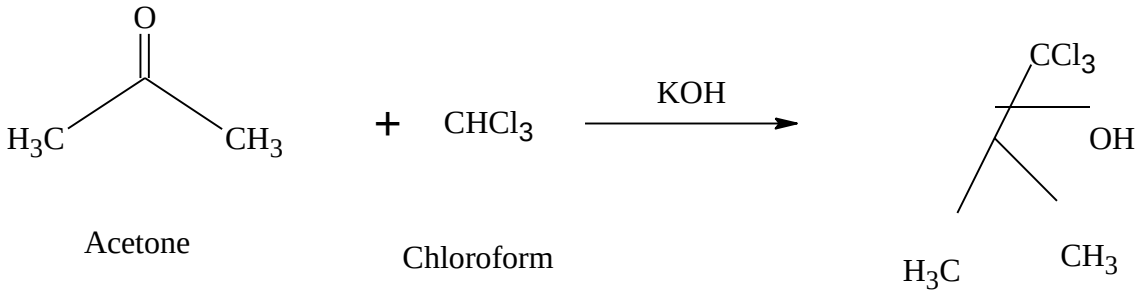
Aim:

To Prepare and submit chlorbutanol from acetone and calculate the Percentage Yield.

Principle:

Chlorbutanol is also known as Chloroketone. It is a trichloro derivative oftertiary butyl alcohol. It is prepared by combination with acetone and chloroform in the presence of solid potassium hydroxide Chlorobutanol is used as local anaesthetic in dental preparation and also antiseptic.

Reaction:



Acetone + Chloroform → Chlorbutanol

Chemical Required:

Chloroform – 11 ml

Potassium hydroxide – 1 gm

Acetone – 14 ml

Procedure:

About 11 ml of chloroform and 1 gm of solid potassium hydroxide are taken in a round bottom flask shake until the potassium hydroxide dissolves. To this 14 ml of acetone was added and shaken for 15 minutes. Then set aside for half an hour and crystal of chlorbutanol was separated out.

Melting Point: 95°C – 99°C

Use:

Local anaesthetics

Report:

Chlorbutanol was Prepared and submitted and reported the following

1. Theoretical Yield =
2. Practical Yield =
3. Percentage yield =

Experiment No: 04

Synthesis of Tolbutamide

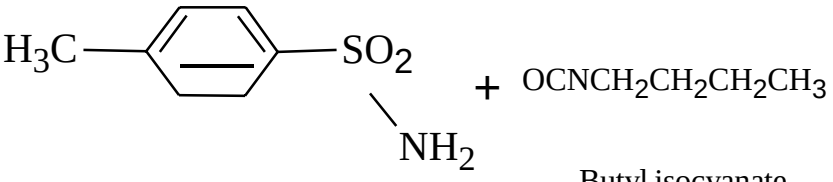
Aim:

To prepare and submit tolbutamide from p-toluene sulfonamide andcalculate its percentage yield.

Principle:

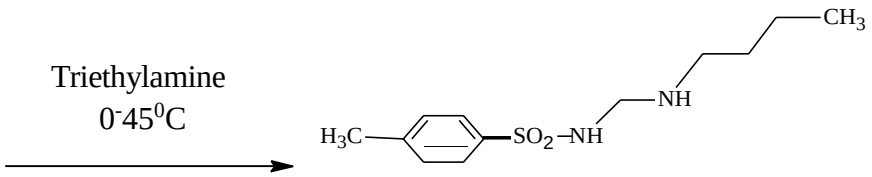
The synthesis of tolbutamide involves addition reaction of p-toluene sulfonamide and butyl isocyanate in the presence of triethylamine and tetrahydrofuran.

Reaction:



P Toluene Sulphonamide

Butyl isocyanate



Tertrahydrofuran

Tolbutamide

Chemical Required:

p-Toluene Sulfonamide – 1 g

Butyl isocyanate – 1 g

Triethylamine – 1.2 ml

Tetrahydrofuran – 10 ml

Procedure:

About N-butyl isocyanate (1m mol) and triethylamine (1.2m mol) in a round bottom flask containing 10 ml of tetrahydrofuran, kept in an ice bath. To the above mixture P-toluene sulfonamide (1m mol) was added drop wise at 0oc. After completing the addition, the temperature was suddenly raised to 35-45oC

and stirred for 3-4 Hrs. Then the solution was filtered. The product wasseparated and dried. Then it was recrystalised by using Diethyl ether.

Melting Point: 128^{o}C to 129^{o}C

Use:

Anti-diabetic

Report:

Tolbutamide was Prepared and submitted. Report the Following

Theoretical Yield:

Practical Yield: Percentage

Yield:

Experiment No: 05

Synthesis of Hexamine

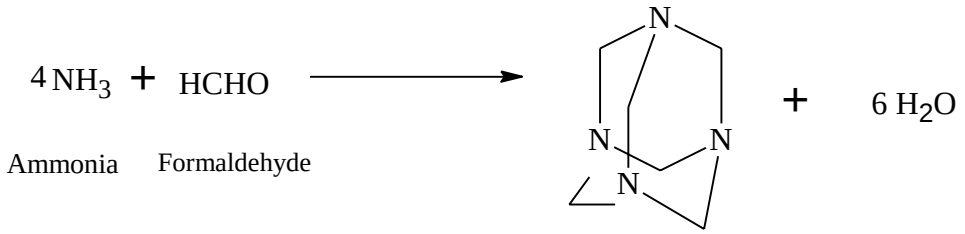
Aim:

To prepare and submit hexamine from formaldehyde and calculate it'sPercentage Yield.

Principle:

Hexamine is heterocyclic organic compound $(CH_2)6N_4$. It has symmetrical tetrahedral cage-like structure. It is prepared by condensationreaction between formaldehyde and ammonia.

Reaction:



Hexamine

Chemical Required:

Formaldehyde – 4.7 g

Ammonia Solution – 7 g

Procedure:

About 4.7g of 30% formaldehyde solution was taken in a beaker and add 7g of 24% ammonia solution, until the solution is slightly alkaline. The mixture was heated on a water bath for 5 minutes and allowed to stand for 15 minutes. The solution was filtered and then evaporated on a direct flame using china dishto a thick paste. The hexamine crystals are obtained and dried. It was recrystallized from water or alcohol. Hexamine forms colourless, odourlesscrystals, which are soluble in water and 90% alcohol.

Use:

Urinary anti-infective agent

Report:

Hexamine was prepared and submitted. Report the following

Theoretical Yield:

Practical Yield: Percentage

Yield:

Experiment No: 06

Assay of Isonicotinic acid hydrazide

Aim:

To determine the percentage purity of given sample of Isonicotic acidhydrazide tablet.

Principle:

Isonicotinic acid hydrazide/ isoniazid is an anti-tubercular drug. It isassayed by the direct titration of Potassium bromate with addition of potassium bromide in the presence of acid medium using hydrochloric acid. During oxidation reaction liberated bromine reacts with isoniazid in aqueous solution toform isonicotinic acid. Azo dye methyl red indicator is used in this titration, decolorized the red colour is the end point.

Reaction:

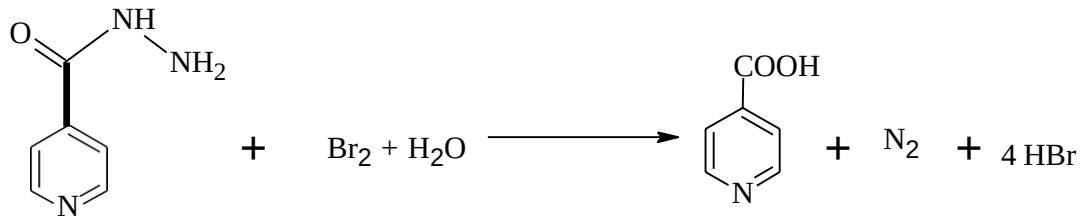
Standardisation:

$$KBrO_3 + 6\,KI + 6\,HCl \longrightarrow KBr + 6\,KCl + 3I_2 + 3\,H_2O$$

$$I_2 + 2\,Na_2S_2O_3 \longrightarrow Na_2S_4O_6 + 2\,NaI$$

Assay:

$$KBrO_3 + 5KBr + 6\,HCl \longrightarrow 3Br_2 + 6\,HCl + 3H_2O$$



Isonicotinic acid hydrazide

Isonicotinic acid

Procedure:

Preparation of 0.0167 M Potassium bromate solution:

About 5.566gm of Potassium bromate was dissolved in water and madeup to 1000 ml with distilled water.

Standardisation of 0.0167 M Potassium bromate:

20 ml of above solution was transferred in a glass stopper flask and 3 g ofPotassium iodide and followed with 3 ml of HCl was added. Allow to stand for5 min, titrate liberated Iodine with 0.1 M sodium thiosulphate adding 3 ml of starch solution TS and the end point is approached.

$$\text{Concentration of 0.0167 M Potassium bromate} = \frac{\text{Molarity of Sodium thiosulphate}}{\text{Volume of Potassium bromate}}$$

Assay of Isonicotinic acid hydrazide tablet

Twenty tablets were weighed accurately and pulverized. A weighed quantity of the tablet power equivalent to 0.25 mg INH was transferred into a clean and dry 100 ml volumetric flask, then sufficient water was added to produce 100 ml. 20 ml of above solution was taken. Then 100 ml of water, 20ml of hydrochloric acid and 0.2 gm of Potassium bromide were added. Then titrated against slowly with continuous shaking with 0.0167M potassium bromate using 0.05ml of methyl red as an indicator until red colour disappears.

Each ml of 0.0167M Potassium bromate KBrO3 = 0.003439g of $C_6H_7N_3O$.

Report:

The Molarity of 0.1 M Sodium nitrite

The percentage purity of given isonicotinic acid Hydrazide tablet wasfound to be:

Experiment No: 07

Assay of Metronidazole

Aim:

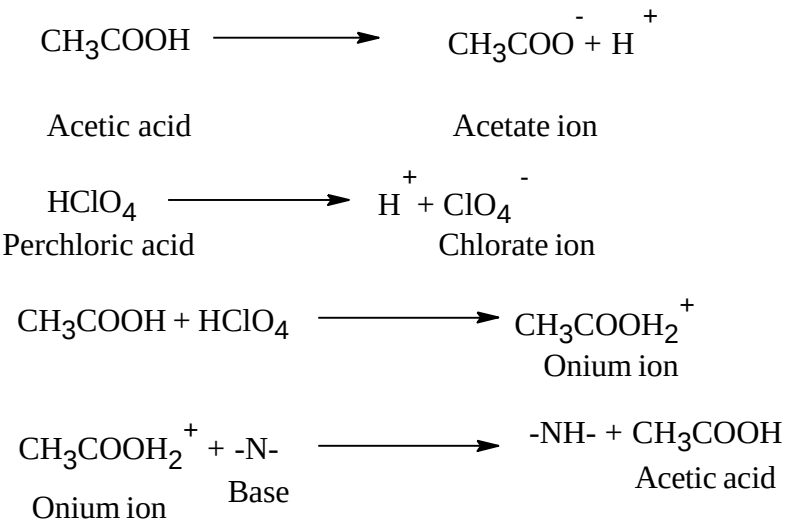
To determine the percentage purity of given sample of Metronidazole tablet.

Principle:

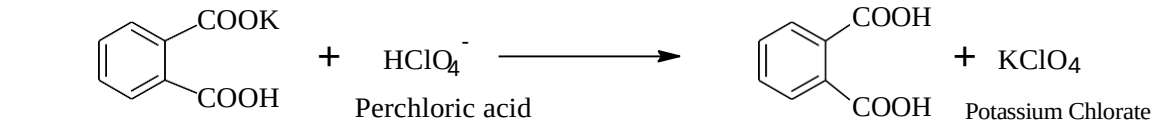
Substance with very weak acid or basic property do not give sharp end point in aqueous solution can be titrated with non-aqueous solvents. Non- aqueous titration is based on Bronsted-Lowry theory According to this theoryan acid is a proton donor, i.e. a substance which tends to dissociate to yield a proton, and a base is proton acceptor, i.e. a substance which tends to combine with a proton. When an acid HB dissociates it yields a proton together with the conjugate base B of the acid.

Metronidazole is a weak base and it is assayed by non-aqueous titration. When a weakly basic drug is dissolved in acidic solvent with titration of perchloric acid, the basic property of mineral is enhanced. If a strong acid like perchloric acid is added in acetic acid, the acetic acid behaves as a base and combine with proton donated by perchloric acid to form onium ion which act as strong acid, the onium ion is readily donates the proton to the base. The indicator used in this titration is crystal violet. The use of acetic anhydride in this solution, it combines with the water molecule to form acetic acid.

Reaction:



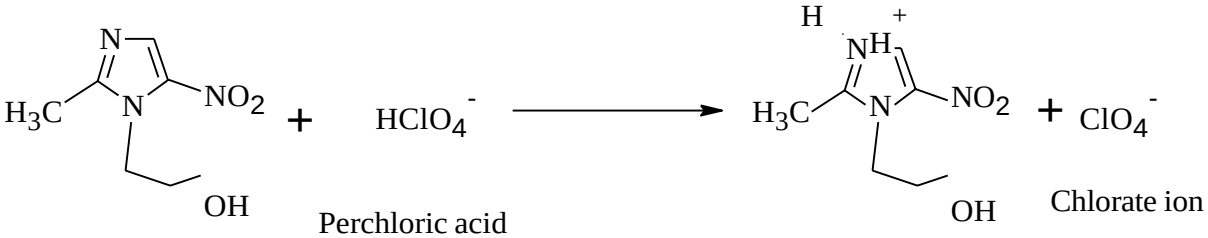
Standardisation:



Potassium Hydrogen phthalate

Phthalic acid

Assay:



Metronidazole

Conjugate acid of Metronidazole

Procedure:

Preparation of Perchloric acid 0.1M

Mixed 8.5 ml of Perchloric acid in 900 ml of glacial acetic acid shake vigorously and continuous stirring. Then added 30 ml acetic anhydride andmake up the volume to 1 litre with glacial acetic acid and allowed to stand for24 Hours before use. The acetic anhydride reacts with the water in perchloric acid and some traces in glacial acetic acid thereby making the resulting mixture practically anhydrous.

Standardisation of 0.1 N Perchloric acid

About 0.5g of Potassium hydrogen phthalate were weighed accuratelyand transfer in a 100 ml conical flask, previously dried at 120^{o}C for 2 hours. 50ml of glacial acetic acid was added, warmed if necessary, to dissolve the salt completely. Cooled and titrated with 0.1M perchloric acid using crystal violet 0.1ml (2 drops) as an indicator. The end point is colour changes from violet to emerald green.

Each ml of 0.1M Perchloric acid = 0.02042g of Potassium hydrogen Phthalate

Assay of metronidazole:

About 3.0g of metronidazole sample was weighed accurately and transfer into a 250ml conical flask, 50ml of Glacial acetic acid was added, warmed gently. Cooled and titrated with 0.1M perchloric acid using α-Naphthol benzeneas an indicator. The end point is colour changes from Blue to Blue-green.

Each ml of 0.1M perchloric acid = 0.02042g of Potassium hydrogen Phthalate.

Report:

The Molarity of 0.1M Perchloric acid=

The Percentage purity of given metronidazole was found to be=

Experiment No: 08

Assay of Dapsone

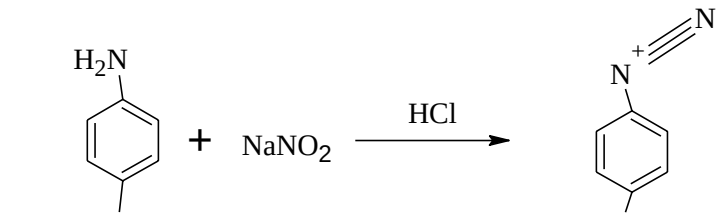
Aim:

To determine the percentage purity of given sample of tablet.

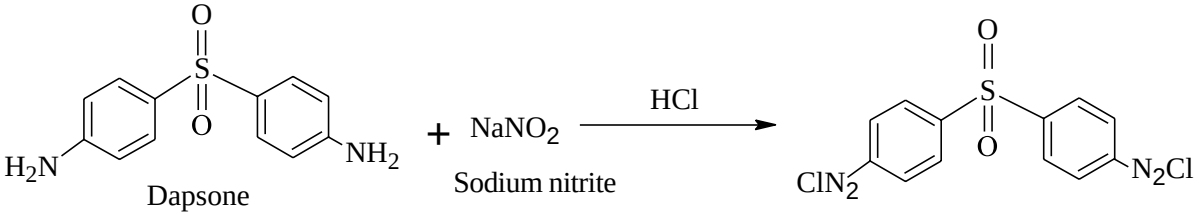
Principle:

Dapsone is a diamino diphenyl sulphone. It is assayed by direct diazotization titration. The free primary amino group present in dapsone is diazotized by nitrous acid and hydrochloric acid to form arene diazonium compound. The end point can be determined by using external indicator i.e. starch iodide paper, during titration with sodium nitrite an aromatic primary amine is diazotized. After the end point the drug solution containing a slight excess of nitrite comes in contact with starch iodide paper. It oxidizes iodideinto iodine which gives blue colour with starch indicating the end point.

Reaction:



Sulphanilic acid — Diazonium ion



Dapsone — Sodium nitrite — Diazonium salt

Procedure:

Preparation of 0.1M Sodium nitrite solution:

7.5g of sodium nitrite was dissolved in sufficient water to produced 1000ml.

Standardisation of 0.1M Sodium nitrite:

0.3g of sulphanilic acid was dissolved in 50ml of 2M hydrochloric acid, 3g of potassium bromide was added, cool in ice and titrate with 0.1M sodium nitrite solution using starch iodide paper as external indicator.

Each ml of 0.1M Sodium nitrite= 0.01732g of $C_6H_7NO_3S$.

Assay of Dapsone tablet:

20 tablets were weighed and powered. Tablet powder equivalent to 0.25gm dapsone was weighed and dissolved in a mixture of 15ml of 2M hydrochloric acid. The solution was cooled to about 15^oC and carry out sodium nitrite titration using starch iodide paper as an external indicator. End point is immediate appearance of blue colour.

Each ml of 0.1M sodium nitrite= 0.01241g of $C_{12}H_{12}N_2O_2S$.

Report:

The Molarity of 0.1M sodium nitrite=

The percentage purity of given dapsone tablet was found to be=

Experiment No: 09

Assay of Chlorpheniramine Maleate

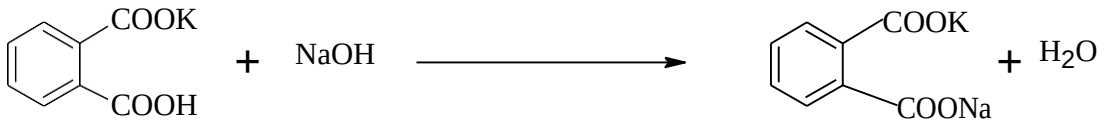
Aim:

To determine the percentage purity of given sample of Chlorpheniraminemalate.

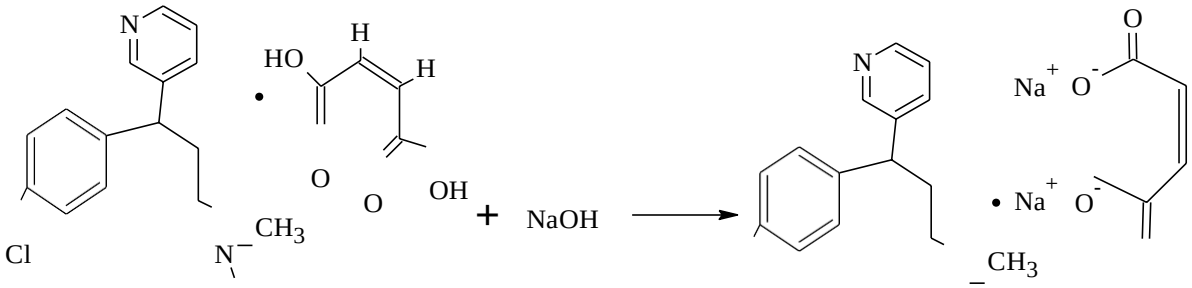
Principle:

Chlorpheniramine maleate chemically known as 3-(4-chlorophenyl) N, N- Dimethyl-3-(2-pyridyl) propylamine hydrogen maleate is an anti-histamine H1 receptor antagonist. Mineral acid salts of weak nitrogen bases hydrolyse so extensively in aqueous or hydro-alcoholic solution that is possible to titrate the liberated acid with a strong mineral base. Titration of the maleate salt of thedrug in water against the sodium hydroxide leads to the formation of water turbidity as the titration proceeds. To prevent this precipitation, alcohol has been used. Since alcohol is basic with respect to water as a solvent, dissolved bases react less strongly alkaline, their salts react more strongly acid, and the end points of the titrations are greatly sharpened, here an aqueous solution of Chlorpheniramine maleate was titrated with aqueous NaOH, the turbidity was formed with appearance of pink is the end point.

Reaction:



Potassium hydrogen phthalate — Sodium salt



CH_3

Chlorpheniramine maleate

Chlorpheniramine disodium maleate

+ 2 H_2O

Procedure:

Preparation of 0.01M Sodium hydroxide:

Weighed accurately about 0.4gm of Sodium hydroxide pellet in a clean 1000ml standard flask then completely dissolved with 100ml distilled water, and make up to 1000 ml with distilled water.

Standardisation of 0.01M sodium hydroxide:

Weighed accurately about 0.5gm of potassium hydrogen phthalate and transferred into 1000ml conical flask. Then add 75ml of distilled water todissolve and titrated with 0.01M sodium hydroxide solution using 0.1ml phenolphthalein as an indicator. The end point is appearance of permanent pale pink colour.

Each ml of 0.01M Sodium hydroxide= 0.002042g of $C_8H_5KO_4$

Assay of Chlorpheniramine maleate

Twenty tablets were weighed and grind into a fine powder. An amount of power equivalent to 200mg of chlorpheniramine maleate was weighedaccurately into 100ml standard flask, 70ml of neutral alcohol was added and shaken for about 20 min. Then, the volume was made up to mark with neutral alcohol, mixed well and filtered using whatmann No 42 filter paper. The first 10ml portion of the filtrate was discarded. An aliquot of the drug solution containing 2.0-20.0 mg of chlorpheniramine maleate was measured accurately and transferred into a clean 100 ml conical flask and the total volume was brought to 10 ml with neutral alcohol. Then 2 drops of 0.5% phenolphthalein indicator was added and the solution was titrated with standard 0.01M Sodium hydroxide solution until a permanent pink colour was obtained.

Each ml of 0.01M Sodium hydroxide= 0.002042g of $C_8H_5KO_4$.

Report:

The molarity of 0.01M Sodium hydroxide=

The percentage purity of given Chlorpheniramine maleate tablet wasfound to be=

Experiment: 10

Assay of Benzyl Penicillin

Aim:

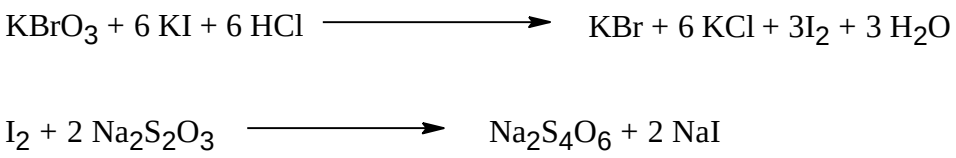
To determine the percentage purity of given sample of Benzyl penicillin tablet.

Principle:

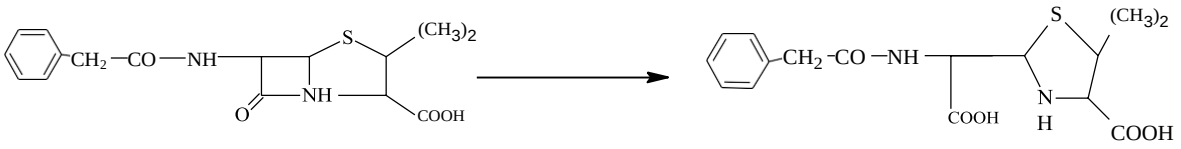
Benzyl penicillin is assayed by iodometric titration method. The titration in which equivalent amount of iodine is liberated to form potassium iodide by the sample and the liberated iodine is titrated against standard sodium thiosulphate solution. This type of indirect titration determination of compoundsis called iodometric titration. In this titration benzyl penicillin is first hydrolysed with sodium hydroxide solution converted to corresponding penicilloic acid (dicarboxylic acid). Then penicilloic acid further treated with mineral acid to form D-Penicillamine and benzyl penicillic acid. An obtained D-penicillamine is further oxidized quantitatively iodine to give disulphide, excess of iodine is back titrated with 0.02M sodium thiosulphate, equivalent amount of liberated iodine can be measured by titration with sodium thiosulphate using starch as an indicator, which is added near the end point as it get hydrolysed by hydrochloricacid and iodine gets trapped in the matrix of starch. Due to this there is no continuous liberation of iodine. An end point is blue to apple green.

Reaction:

Standardisation:

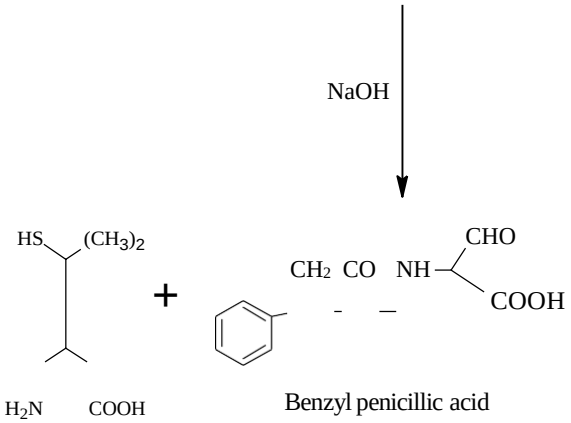


Assay:



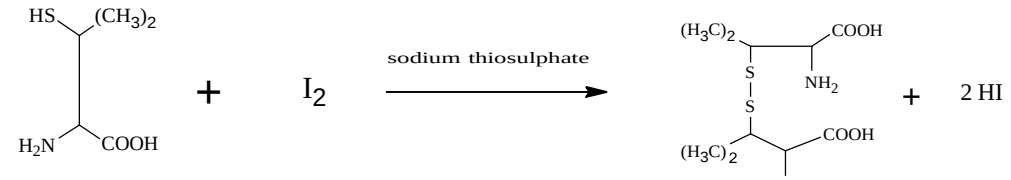
Benzyl penicillin

Penicilloic acid



D penicillamine

Benzyl penicillic acid



D penicillamine

NH_2

Procedure:

Preparation of 0.02N Sodium thiosulphate:

0.02N sodium thiosulphate (4.564 gm of sodium thiosulphate and 250 mgof sodium carbonate) dissolved in 100 ml of water then make up to 1000ml withwater.

Standardization of 0.02N sodium thiosulphate:

Dissolved accurately weighed 0.2g of potassium bromate in 250ml of water taken in a conical flask. From this take 50 ml of the solution, add 2g of potassium iodide, 3ml of 2M HCl and titrate with sodium thiosulphate solution using starch as an indicator until the blue colour is discharged.

Each ml of 0.01N sodium thiosulphate= 0.002784g of KBr.

Assay of Benzyl penicillin:

Weighed accurately about 0.1gm of sodium salt of benzyl penicillin takenin a stoppered flask, dissolved in 10ml of water and dilute to 100ml. 10ml of solution was transferred into iodine flask, 5ml of 1N sodium hydroxide was added, allowed to stand for 20 minutes. Then freshly prepared buffer solution, 5ml of 1N hydrochloric acid and 25ml of excess of 0.02N iodine solution were added to the stoppered flask and kept aside for 20 minutes in a dark place. Excess of iodine is titrated with 0.02N sodium thiosulphate using freshly prepared starch solution as an indicator. The end point is discoloration of blue colour. To another 10ml of initial solution add 20ml of the buffer solution, allowed to stand for 20 minutes in the dark place and titrate with the same. The difference between two titration represents the volume of 0.02N iodine equivalent to the total amount of penicillin present in the given sample ofbenzyl penicillin.

Report:

The molarity of 0.01M sodium thiosulphate=

The percentage purity of given Benzyl penicillin tablet was found to be=

Experiment No: 11

Synthesis of Phenytoin from Benzil by Microwave Irradiation

Aim:

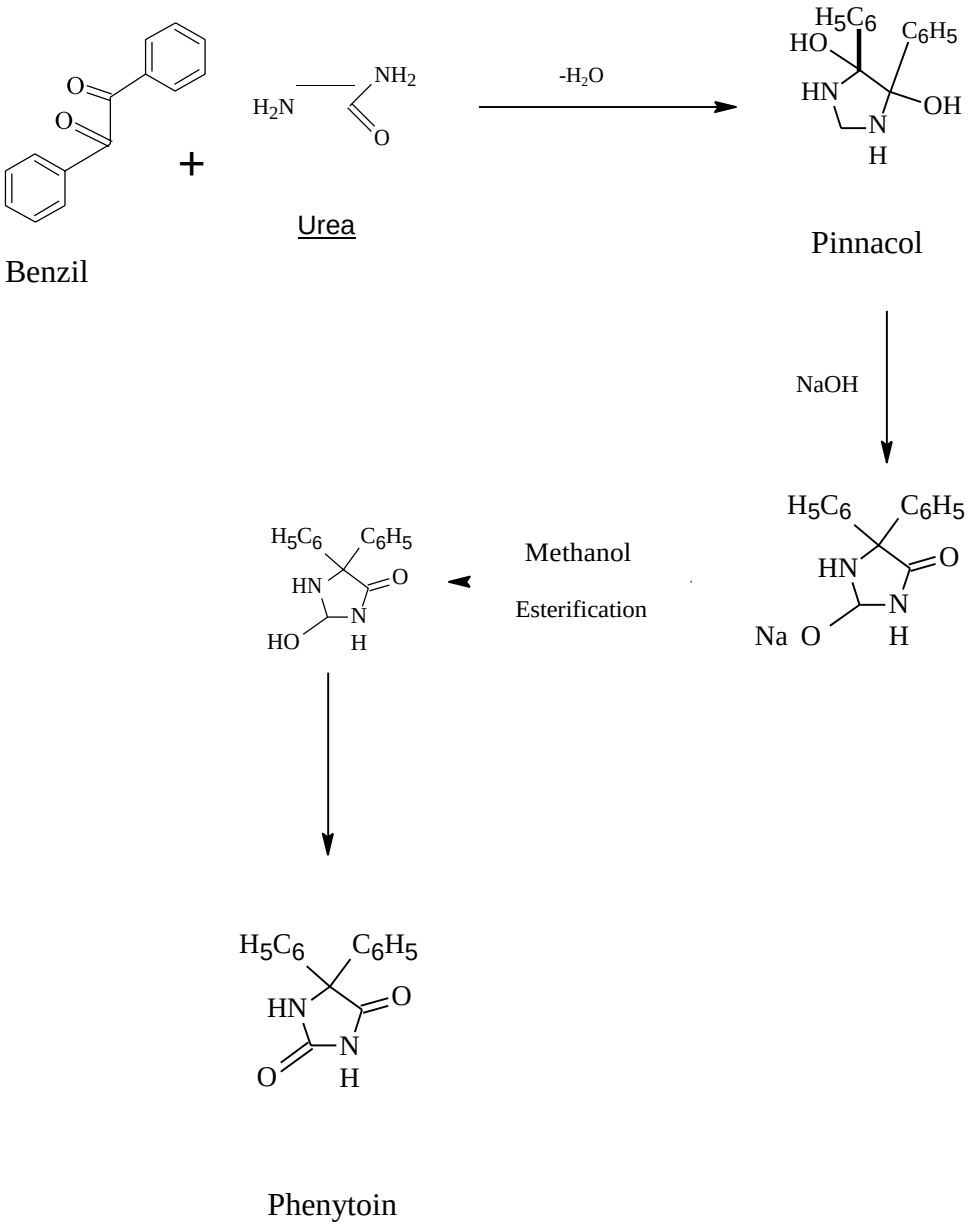
To synthesis and submit phenytoin from benzil by using microwave oven and calculate its percentage yield.

Principle:

The microwave region of Electro Magnetic spectrum light between IR irradiation and frequency corresponding to the wavelength of $1cm^{-1}$ to 1m. The organic compound can be heated by applying energy in the form of microwave high frequency IR irradiation. The use of this technique can have substantial saving time for laboratory synthesis of drugs and chemicals.

Phenytoin is prepared by condensation of benzil and urea under reflux condensation to give heterocyclic compound Pinnacol. When the pinnacol is treated with sodium hydroxide it's rearrangement to produce phenytoin as sodium salt and the esterification gives phenytoin as crude product. This reaction is completed to take place only 2 to 3 minutes microwave irradiation.

Reaction:



Chemicals Required:

Benzil = 1.25g

Urea = 0.75g

NaOH (30%)= 3.75 ml

Methanol = 18.75 ml

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Procedure:

1.25gm of benzil, 0.75gm urea, 3.75ml 30% sodium hydroxide and 18.75 ml methanol was taken in a beaker and kept in a Microwave oven for 3 minutes.Then it was cooled to room temperature and 50ml of water was poured, mixed well and filtered. To the filtrate con. HCl, was added to get the crude product. Then the product was recrystallized from ethanol.

Melting Point: 295^{o}C to 298^{o}C

Use:

Anti-convulsant

Report:

Phenytoin was synthesised and reported the following

1. Theoretical yield =
2. Practical yield =
3. Percentage yield =

Experiment No: 12

Synthesis of Aspirin Assisted by Microwave Oven

Aim:

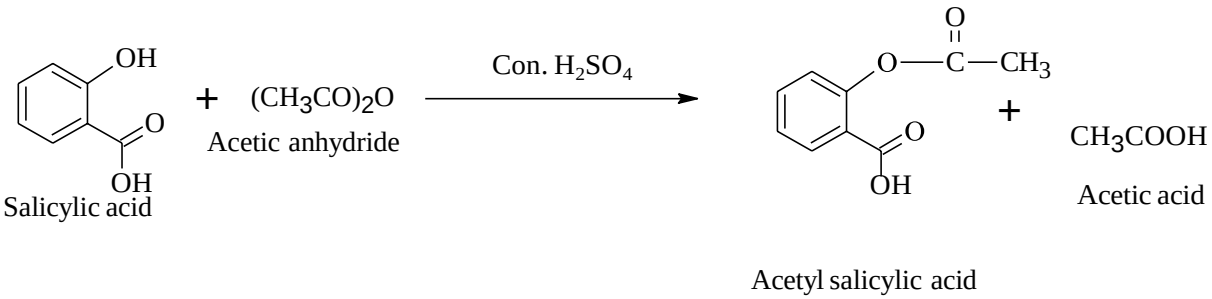
To Prepare and Submit aspirin from Salicylic acid and Calculate the Percentage Yield.

Principle:

The microwave region of Electro Magnetic spectrum light between IR irradiation and frequency corresponding to the wavelength of 1cm-1 to 1m. The organic compound can be heated by applying energy in the form of microwave high frequency IR irradiation. The use of this technique can have substantial saving time for laboratory synthesis of drugs and chemicals.

Aspirin is prepared from Salicylic acid, in this method salicylic acid reactwith acetic anhydride in the presence of sulphuric acid to form crystalline natureof aspirin.

Reaction:



Salicylic acid

Acetyl salicylic acid

Procedure:

Two reaction consist of a two-neck flask with magnetic stir bar, temperature, sensor and intensive cooler. A mixture of salicylic acid and acetic anhydride is filled in the reaction flask and three drop of conc. Sulphuric Acid are added the apparatus is installed by means of a glass tube in the microwave system. Standard refluxing apparatus for microwave system. The reaction mixture is heated under stirring for 90 sec. with 900 W to 140 C, during the following cooling down the clear yellowish solidified to a compact white crystalline mass.

Melting Point: 135^0C

Use:

Anti-inflammatory agent

Result:

Aspirin was synthesised and reported the following

1. Theoretical yield =
2. Practical yield =
3. Percentage yield =

Experiment No 13:

Drawing structure and Reaction using Chemsketch

CHEM SKETCH

ACD/ChemSketch is a molecular modeling program used to create and modify images of chemical structures. Also, there is a software that allows molecules and molecular models displayed in two and three dimensions, to understand the structure of chemical bonds and the nature of the functional groups.

The program offers some advanced features that allows the molecules rotate and apply colour to improve visualization. It has several templates with ions and functional groups with the possibility to add text and use other tools to optimize productions created by the software.

Application

Using ACD/ChemSketch is primarily for educational use. With this program it is possible to write and perform chemical equations, diagrams laboratories and chemical structures of various entity.

Computational chemistry software		
Cheminformatics	Open-source	❖ Avalon Cheminformatics Toolkit ❖ Bioclipse ❖ Blue Obelisk ❖ Chemistry Development Kit ❖ ECCE ❖ JOELib ❖ OELib ❖ Open Babel ❖ RDKit
	Proprietary	❖ Canvas ❖ Chemicalize ❖ Discovery Studio
Chemical kinetics	Open-source	❖ APBS ❖ Cantera ❖ KPP
	Proprietary	❖ Autochem ❖ Chemical WorkBench ❖ CHEMKIN ❖ COSILAB ❖ DelPhi ❖ Khimera

Molecular modelling visualization	Open-source	❖ Ascalaph Designer ❖ Avogadro ❖ BALL ❖ Biskit ❖ CPMD ❖ Gabedit ❖ Ghemical ❖ Jmol ❖ Molekel ❖ PyMOL ❖ QuteMol ❖ RasMol
	Proprietary	❖ Abalone ❖ ACD/ChemSketch ❖ Atomistix ToolKit ❖ ChemDraw ❖ ChemWindow ❖ EzMol ❖ Gaussian ❖ Maestro ❖ MarvinSketch ❖ MarvinView ❖ MODELLER ❖ MolecularOperating Environment ❖ SAMSON ❖ Spartan ❖ UCSF ❖ Chimera ❖ VMD
Molecular docking	Open-source	❖ AutoDock ❖ AutoDock Vina ❖ FlexAID ❖ rDock
	Proprietary	❖ Glide ❖ LeDock ❖ Molecular Operating Environment
Molecular dynamics	Open-source	❖ CP2K ❖ GROMACS ❖ LAMMPS ❖ OpenMM ❖ PLUMED
	Proprietary	❖ Abalone ❖ AMBER ❖ CHARMM ❖ Desmond ❖ GROMOSNAMD

Quantum chemistry	Open-source	❖ ABINIT ❖ ACES(CFOUR) ❖ AIMAll ❖ BigDFT ❖ CP2K ❖ DACAPO ❖ Dalton ❖ DP code ❖ FreeON ❖ HORTON ❖ MADNESS ❖ MPQC ❖ NWChem ❖ Octopus ❖ PARSEC ❖ PSI ❖ PyQuante ❖ PySCF ❖ Quantum ESPRESSO ❖ (PWscf) ❖ RMG ❖ SIESTA ❖ VB2000 ❖ YAMBO code
	Proprietary	❖ ADF ❖ AMPAC ❖ DMol3 ❖ CADPAC ❖ CASINO ❖ CASTEP ❖ COLUMBUS ❖ CONQUEST ❖ CPMD ❖ CRUNCH ❖ CRYSTAL ❖ DIRAC ❖ Firefly ❖ GAMESS (UK) GAMESS (US) ❖ Gaussian ❖ Jaguar ❖ MOLCAS ❖ MOLPRO ❖ MOPAC ❖ ONETEP ❖ OpenAtom ❖ ORCA ❖ PLATO ❖ PQS

		❖ Q-Chem ❖ Quantemol ❖ Scigress ❖ Spartan ❖ TeraChem ❖ TURBOMOLE ❖ VASP ❖ WIEN2k ❖ XMVB
Skeletal Structure drawing	Open-source	❖ BKChem ❖ JChemPaint ❖ JME Molecule Editor ❖ Molsketch ❖ XDrawChem
	Proprietary	❖ ACD/ChemSketch ❖ ChemDoodle ❖ ChemDraw ❖ ChemWindow ❖ MarvinSketch
Others		❖ Aqion ❖ Eulim ❖ EXC code ❖ GenX ❖ GSim ❖ ICM (ICM-Browser) ❖ Materials Studio ❖ Molden ❖ OpenChrom ❖ RubyChem ❖ SASHIMI