RAYS

Academic Insights of Morning Star

Morning Star Home Science College,
Angamaly

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MORNING STAR HOME SCIENCE COLLEGE, ANGAMALY

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Editorial

"Research is to see what everybody else has seen, and to think
what nobody else has thought."

-AlbertSzentGyorgyi

As this first edition of RAYS comes out in print, I am extremely delighted to pen a few words of acknowledgement and encouragement for the contributions made by our teachers and students towards the field of scientific study and research. I congratulate the teachers for instilling their students' minds with an aptitude for research and inquisitiveness to understand working principles, explore scientific phenomenon and make calculated deductions. This platform will serve as a source of motivation for teachers and students to delve into research and bring their work out in print for others to be enriched.

I thank everyone who has contributed to this cause and congratulate all the teachers and students for their enthusiastic research and dedicated hard work. I invite your continued support and contribution of article/research papers on science. May the good Lord bless you all.

Best wishes,

Dr. Sr. Rosily A. V.
Chief Editor

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Microscale experiments in chemistry

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Abstract

The current work aims to study the feasibility of microscale experimental techniques in undergraduate level chemistry practical sessions. It involves the application study of microscale techniques to the physical chemistry (determination of partition coefficient of iodine between carbon tetrachloride and water), in qualitative inorganic mixture analysis and also in organic qualitative analysis.

Introduction

The crucial role of practical work and experimentation in science curriculum is universally accepted. This is more so in chemistry which is an experimental science. However, there are certain factors which contribute to the marginalization of various important experiments in colleges and universities. Performing experiments on large scale constituting the traditional methods employed in undergraduate and postgraduate labs involves cumbersome assembly of apparatus, use of large quantities of chemicals, outlet of synthesized product ,excess reagents and solvents that pollute the environment, evolution of large amount of toxic gases that pose health hazards to students, teachers and lab staffs.

Alternative ideas to replace the conventional laboratory setups while meeting the objectives of practical work are being thought of. Recent developments introduce microscale chemistry experiments which use small quantities of chemicals and simple equipment. Microscale experiments involve much more new, advanced, interesting and easy going laboratory techniques which are not at all harmful. Microscale chemistry is a student friendly as well as an environment friendly chemistry. Researches and studies have proven that there will be wide applications of micro scale chemistry in the coming years. The concept of micro scale chemistry was first introduced by D.W. Mayo and S.S. Butcher at Bowdoin College in Brunswick about 30 years ago.

Microscale chemistry

Reduction of chemical use to the minimum level at which experiments can be effectively performed is known as Microscale Chemistry. Microscale chemistry is environmentally safe pollution prevention method of performing chemical processes using small quantities of chemicals without compromising the quality and standard of chemical applications in education and industry. It creates a sense of 'Green Chemistry'.

Microscale chemistry is performed by using drastically reduced amounts of chemicals, safe and easy manipulated techniques and miniature lab ware and high quality skills. Microscale chemistry amounts to a Total Quality Management (TQM) approach to the use of chemicals. Microscale chemistry is recognized as small

scale chemistry by the International Union of Pure and Applied Chemistry.

Nowadays microscale experiments are widely conducted in colleges and universities. While much of traditional chemistry centers on milligrams preparation, milligrams of substances are only required for microscale chemistry.

Advantages of microscale chemistry experiments

1. They aremost economical and speedy.
2. They involve the use of extremely small quantities of chemicals (10mg or less).
3. They save time for preparation of reactants and require only shorter experiment time.
4. They reduce chemical use promoting waste reduction at the source.
5. They are safer.
6. They lower costs for chemicals and equipments thus sharply reducing the laboratory cost.
7. They are environmental friendly.
8. They require only smaller storage area.
9. They involvepleasant working atmosphere.
10. They requireonly shorter reaction time.
11. They have reducedreliance on intensive ventilation.
12. They improve laboratory skills of students and they are more Student friendly.
13. They provideclean and productive environment.
14. They lowerglass breakage cost.
15. They offer vastly improved laboratory safety by:

a. Least exposure to toxic chemicals.

b. No fire and explosion hazards.

c. No spills and accidents.

Experimental methods

The project under study involves three experiments in UG Chemistry practical syllabus. One from physical chemistry, second from inorganic chemistry and the other from organic chemistry. Physical chemistry experiment is the determination of partition coefficient of I_2 between CCl_4 and H_2O. The inorganic chemistry experiment involves qualitative mixture analysis and the organic chemistry experiment involves organic qualitative analysis.

Requirements

1) For the determination of partition coefficient of I_2 between CCl_4 and H_2O

a) Culture bottle

b) Magnetic stirrer

c) Micropipette

d) Boiling tube

e) I_2 in CCl_4

f) 0.001 N & 0.1 N Sodium thiosulphate

g) 10% KI & Starch.

2) For qualitative inorganic mixture analysis.

a) Apparatus like micro level or semi micro level beakers, test tubes and droppers.

b) Milligram levels of the given mixture are taken for each test.

3) For organic mixture analysis.

a) Apparatus like micro level or semi micro level beakers, micro test tubes and droppers.

b) Milligram levels of the given mixture are taken for each test.

Experiments and Experimental Methods

Determination of partition coefficient of iodine between carbontetrachloride & water

Partition coefficient is defined as the

ratio between concentrations of a compound in a mixture of two immiscible phases at equilibrium. This ratio is therefore a measure of the difference in solubility of the compound in these two phases. The two phases are generally solvents. One of them is aqueous (hydrophilic) and the other is organic (hydrophobic).Hence the partition coefficient also measures how hydrophilic or hydrophobic a chemical substance is.

Partition coefficient experiments often involve chemicals like iodine in carbon tetrachloride which are highly expensive and hazardous. The experiments also require good skills to receive accurate results. Much time is also required to conduct the experiments carefully. Partition coefficient experiments also involve steps like mouth pipetting which is dangerous. However, conducting these experiments in micro scale helps to solve the concerned problems as it uses minimum quantity of chemicals and safe equipment's like micropipettes which do not involve mouth pipetting. In addition sharp results are obtained too.

Procedure: Take 12ml in ccl_4 and 6ml H_2O in a culture bottle. Place a small magnetic needle in it. Place it in a magnetic stirrer for 3 minutes. Then place it in a water bath for 5 minutes to attain equilibrium.

Titration 1: Using a micropipette take 1ml from aqueous layer to a boiling tube. Add 0.5ml 10% KI and 2 drops of starch. Titrate against 0.001N thiosulphate {X1}.

Titration 2: Remaining solution (2ml organic solution + 5ml aqueous layer) as a whole is taken. Add 1ml 10% KI + 2 drops of starch solution. Titrate v/s 0.1N thiosulphate. Endpoint is the disappearance of blue colour. {X2 ml of thiosulphate}.

Calculation

C_1-Concentration of I_2 in aqueous layer.

Volume of aqueous layer taken = 1ml

Volume of thiosulphate = 2.6ml

Normality of thiosulphate = 0.001

N_1 (normality of I_2 in aqueous layer) = $(2.6 \times .001)/1 = 0.0026$

C_2-Concentration of I_2 in organic layer.

Volume correction

$V_1 N_1 = V_2 N_2$

$2.6 \times .001 = V_2 \times 0.1$

1ml (aqueous layer) $V_2 = (2.6 \times .001)/0.1$

$= 0.026$

For 5ml aqueous layer $= 5 \times .026$

$= 0.13$(volume correction)

$X_3 = X_2$ - volume correction

$= 4.8 - 0.13$

$= 4.67$

N_2 = Concentration of I_2 in organic layer

V_2 = Volume of organic layer = 2ml

N_1 = Normality of thiosulphate = 0.1

V_1 = Volume of thiosulphate $(X_2 - V)$

$N_2 = N_1 - V_1/V_2 = (0.1 \times 4.77)/2$

$= 0.2335$

Partition Coefficient K $= C_2/C_1$

$= 0.2335/0.0026$

$= 89.800$

2) microscale experiments in inorganic chemistry

Qualitative inorganic mixture analysis

It may be difficult to make a quantum jump from inorganic macro analysis presently in practice to micro analysis where 1 to 10 mg amounts of chemicals

are used. A semi micro procedure which utilize 10 to 100mg of sample will be a better choice with some new techniques of micro analysis for chemistry core students which involves the analysis of 2 anions is not an easy task. All the difficulties that may arise cannot be foreseen and can be evolved during practical sections and solved in situ. However, we have to make a beginning and the problems associated with the changeover can be rectified with mutual sharing of experiences.

The curriculum for B.Sc. Chemistry core practical deals with inorganic qualitative analysis. There are some strong arguments against inclusion of inorganic qualitative analysis in the syllabus. There are many risks in macro scale qualitative inorganic analysis.

- The toxic effect of hydrogen gas used for the intergroup separation of cations is a healthy risk to students, teachers and laboratory staffs.
- There are complaints of inadequate time for the completion of the practical work.
- It is also complicated that the teachers also fail to inspire the students because of the time nature of the work.

However, there are many solid reasons for the inclusion of inorganic mixture analysis in the syllabus. Many chemical concepts which find a place in textbooks need to be practiced in the laboratory during the mixture analysis. The concept of common ion effect and solubility product made use in the inter group separation is an excellent example

Conversion to a microscale chemistry laboratory programme in mixture analysis is an excellent alternative for the usual methods as it can tackle most of the above mentioned problems to a great extent. The setups require an initial outlay of funds. The important factor in funding the conversion of chemistry programmes to the microscale level is the large savings in decreased chemical, storage, energy and waste disposal costs. At this scale, the experiments do not need normal laboratory glassware but can be performed using simple household materials such as tablet packets, homeo medicine bottles and syringes, fusion tubes etc.

In the conventional method, the anions – fluoride, borate, phosphate, chromate, and oxalate cause unexpected results in cation analysis and therefore need to be removed before the cation analysis. Usually they are removed after group II analysis. Instead of following the elimination scheme for these interfering radicals, micro scale experimental techniques involve an alternative method of analysis which do not require a specific elimination procedure and at the same time chemically quite sound, easier, time saving and interesting. Moreover, the elimination process involves the release of toxic gases and chemicals which are harmful for the students and teachers. Adopting the microscale procedure helps to solve these problems.

The microscale method suggested for the cation analysis without the elimination process is described below:

When the sodium carbonate extract (SCE) is prepared for the analysis of anions, displacement reaction takes place. The anions are converted in to sodium salts while the cations are converted in to insoluble carbonates. Thus by analyzing the residue of SCE, the presence of cations

can be confirmed. The method is full proof only if there is complete displacement reaction during the SCE preparation. This is possible in microscale, since only milligram levels of the mixture and sodium carbonate are taken. To achieve maximum displacement during SCE preparation the following points should be remembered.

The mixture and sodium carbonate should be in the ratio 1:3 by mass.

1) Sodium carbonate should be homogenously mixed with the given mixture before transferring to the beaker.

2) During boiling, water should be added in small increments to keep the concentration of the solution constant.

3) The residue of sodium carbonate extract should be washed with water atleast twice to remove all the adhered anions.

The residue from SCE is dissolved in dil.HCl (if insoluble conc. HCl is used) and used for cation analysis.

The scheme of amixture is given below.

EXPERIMENTS	OBSERVATION	INFERENCE	CHEMISTRY
1. Colour& appearance of the mixture is noted.	Pink	Presence of Co2+, Fe2+.....	Transition metal ions have unpaired electron in the valence shell which can cause d-d transition causing absorption of visible light.
2. SOLUBILITY 5mg of the mixture is warmed with the following solvents in succession.			
• H_2O	Insoluble	Absence of Na+, k+……	
• Dil.HCl	Soluble	Absence of group I metal.	$PbCl_2$ is insoluble in water.
• Dil.HNO_3	Soluble & no precipitate on adding dil.HCl.	Absence of group I metal.	

3.**FLAME TESTS** 1. WITH Conc.HCl 5 mg of the mixture is made into a paste with con.HCl in a watch glass & little of this is shown in the flame.	No red or green colour.	Absence of Cr^{2+}, Sr^{2+}……	
2. WITH Conc. H_2SO_4 5mg of the mixture is made into paste with Con.H_2SO_4 & CaF_2 in a watch glass & a little of this is shown in the flame.	No deep green	Absence of Borate.	
PRELIMINARY TESTS FOR ACID RADICALS 1. ACTION WITH DIL.HCl 5 mg of the mixture is warmed with dil. HCl.	No brisk efferves cence & no gas is evolved.	Absence of carbonate, sulphides & sulphites.	
2.RUBBING TEST 5mg of the mixture is rubbed with dil. H_2SO_4 in a watch glass & note the smell.	No smell of vinegar.	Absence of Acetate. Presence of Oxalate	
5mg of the mixture is boiled with dil. H_2SO_4 to expel all the issuing gases & a pinch of MnO_2 is added.	Brisk effervescence of colourless gas. No reddish brown vapours.	Absence of Nitrate	

3. a) 5mg of the mixture is boiled with con.H_2SO_4.	No greenish yellow gas with pungent smell.	Absence of Chlorides	Oxalates are decomposed to oxalic acid by dil. H_2SO_4.the oxalic acid thus formed has undergone oxidation by MnO_2.
4. 5mg of the mixture is warmed with a little con. H_2SO_4& MnO_2.	No characteristic vapours are evolved.	Absence of chloride, bromide or iodide.	
5. CHROMYL CHLORIDE TEST About 5mg of the mixture is mixed with thrice its weight of solid pot. Dichromate& 5 drops of con. H_2SO_4& heated. The issuing vapours are passed through 1ml water contained in a test tube. To the solution 6 drops of acetic acid & 3 drops of lead acetate are added.	No yellow precipitate.	Absence of chloride.	
6. ETHYL BORATE TEST 5 mg of the, mixture is heated with 10 drops of con.H_2SO_4& 5ml of alcohol. The issuing vapours are burnt.	No green edged flame.	Absence of Borate.	
7. ETHYL ACETATE TEST 5 mg of the mixture is boiled with 0.5ml of con.sulphuric acid & 0.5ml alcohol & poured it into water.	No pleasant fruity smell.	Absence of Acetate	

8. AMMONIUM MOLYBDATE TEST 5 mg of the mixture is boiled with 0.5ml con. Nitric acid & this solution is added to 2ml of ammonium molybdate solution taken in another test tube. .	No yellow precipitate.	Absence of phosphate,arsenite or arsenate.	

Systematic tests for acid radicals

5mg of the substances is mixed with 15mg sodium carbonate in a semi micro beaker &boiled with 5ml distilled water for 10 min, adding distilled water at intervals to make up for the loss of evaporation. The separated filtrate is called sodium carbonate extract & used for further analysis. The separated precipitate is washed with water two times & kept for cation analysis.

1. Colour of the extract is noted.	No colour.	Absence of chromate & Mn.	
2. Dil. HNO_3 & $AgNO_3$ Acidify 5ml of extract with dil.nitric acid and silver nitrate.	No characteristic ppt.	Absence of chloride, bromide or iodide .	
3. To the filtrate from the previous experiment add more silver nitrate followed by ammonium hydroxide drop by drop without shaking.	No yellow, chocolate, brown, red ring.	Absence of phosphate or chromate.	

4. Dil. HCl& $BaCl_2$ The extract is acidified with few drops of dil.HCl& add a few drops of $BaCl_2$ solution.	Absence of phosphate or chromate.	Presence of sulphate.	$BaSO_4$ is formed.
5. To the above ppt. add excess dil. HCl.	White ppt. is insoluble in dil.HCl.	Presence of sulphate is confirmed.	$BaSO_4$ is insoluble in dil.HCl.
6. Two drops of the extract is acidified with dil. HCl boiled, cooled &few drops of zirconyl nitrare or zirconyl chloride reagent is added.	No white gelatinous ppt.	Absence of phosphate is confirmed.	
7. Acetic Acid & $CaCl_2$ Solution Acidify 5 drops of the extract with acetic acid and add $CaCl_2$ solution.	White precipitatewhich decolourises KmnO4 in warm dil.H_2SO_4.	Presence of oxalate is confirmed.	Oxalates are decomposed by H_2SO_4 to produce oxalic acid which being a reducing agent reduces $KMnO_4$.
8.5 drops of the extract is acidified with 5ml dil.Nitric acid, boiled, neutralised with ammonium hydroxide. The excess ammonia is boiled off. To this neutral ferric chloride solution is added	No red colour.	Absence of acetate is confirmed.	

9. BROWN RING TEST 5 drops of the extract is acidified with 2ml dil. sulphuric acid & mixed with 5 drops of freshly prepared ferrous sulphatesolution, then add 1ml con. Sulphuric acid along the sides of the test tube without shaking.	No brown ring.	Absence of nitrate is confirmed.	

From the analysis it is confirmed that the given mixture containing the following anions – OXALATE AND SULPHATE.

Inter group separation of cations

<table>
<tr><td colspan="6">To a little of the solution of the residue obtained after SCE preparation dil. HCl is added drop by drop & centrifuged</td></tr>
<tr><td>No residue</td><td colspan="5">Centrifugate: pass H_2S & centrifuged</td></tr>
<tr><td rowspan="5">Absence of group l cations (pb^{2+})</td><td rowspan="5">No residue. Absence of group llcations (Bi,Cu^{2+})</td><td colspan="4">Centrifugate: boiled off hydrogen peroxide. Then add NH_4Cl & NH_4OH excess & centrifuged.</td></tr>
<tr><td rowspan="4">No residue. absence of group lllcations(Al^{3+},Fe^{2+})</td><td colspan="3">Centrifugate: evaporated to reduce the volume. Add 1-2 drops of ammonia. Then H_2S is added & centrifuged</td></tr>
<tr><td rowspan="3">Residue: white ppt Presence of group lVcations (Co^{2+}, Ni^{2+}….)</td><td colspan="2">Centrifugate: reduce the volume. Add few drops of dil. HCl then NH_4Cl, NH_4OH & $(NH_4)_2CO_3$ added & centrifuged.</td></tr>
<tr><td>No residue: absence of group V.(Sr^{2+},Ca^{2+})</td><td>Centrifugate: evaporated to dryness in a china dish. 2 drops of con.HNO_3 is added. Absence of group Vlcations.</td></tr>
<tr><td></td><td></td></tr>
</table>

Analysis of group lV

The group lVppt is treated with very dil.HCl shaken well & centrifuged		
No residue. Absence of cobalt & nickel	Centrifugate : boiled off H_2S & excess NaOH warm & centrifuged	
	Residue – Presence of Mn^{2+} to a pinch of the residue 5 drops of con.HNO_3& a pinch of PbO_2 are added & boiled. Diluted with water & kept for a few minutes pink colour, presence of Mn^{2+}. Chemistry: Permanganic acid is formed.	Centrifugate: saturate one part with H_2S. Acidify another part with acetic acid & add few drops of pot.ferrocynaide No precipitate- absence of zinc Ash test: the group lVprecipitate is dissolved in dil. Nitric acid & add 2 drops of cobalt nitrate solution. Filer paper dipped in the solution shown to the flame No green ash: absence of zinc is confirmed

Result

From the analysis it is confirmed that the cations present in the given mixture are ammonium & manganese.

3) micro scale experiment in organic chemistry

Organic qualitative analysis

Organic chemistry is the chemistry for the scientific study of structure, properties, and reactions of organic compounds and organic materials (materials that contain carbon atoms). Study of structure determines their chemical composition and formula. Study of properties includes physical and chemical properties, and evaluation of chemical reactivity to understand their behaviour. The study of organic reactions includes the chemical synthesis of natural products, drugs, and polymers.

Qualitative organic analysis of an unknown compound is an integral part of the chemistry curriculum. This type of training is essential as students learn to approach a problem systematically and to interpret the result logically. However, considerable quantities of waste are generated by using conventional methods of analysis. This waste is a complex mixture of compounds, difficult to segregate or reuse, and its commercial disposal incurs a huge expense. Many thousands of undergraduate and postgraduate student study chemistry each year, and at a rough estimate, each student produce about 225g/year of the waste while performing qualitative organic analysis.

Perturbed by these facts, we have made a concerted effort to reduce the quantities of waste generated and to replace the commonly used procedure for organic mixture analysis. The reagents used in the organic qualitative analysis tests are the same as in the conventional analysis and are relatively inexpensive and easily available, in contrast to complex and expensive reagents mention for the organic qualitative analysis tests in the present work have been developed for

the detection of nitrogen and sulphur, Baeyer's test for unsaturation, and the functional groups present in carbohydrate, carboxylic acids, phenols, alcohols, esters, aldehydes, ketones, aromatic nitro compounds, aromatic amides and primary, secondary, and tertiary aromatic amines. The modified scheme is simple, eco-friendly and energy and time efficient.

Experiment

Dicarboxylic acid (phthalic acid)

I PRELIMINARY EXAMINATION		
No residue. Absence of cobalt & nickel	white crystalline solid	may be an acid, amide, or polynuclear hydrocarbon
2.odour	No characteristic odour	May be an acid, amide or carbohydrate
3.solubility	Soluble in dilute sodium hydroxide solution	May be an acid or phenol
4.action on litmus	Turns blue litmus red	Acidic substance
II. DETECTION OF ELEMENTS: LASSGAINE'S TEST		
Preparation of sodium fusion extract		
Fuse metallic sodium metal till silvery. Fuse the organic substance. Cool to room temperature. Keeping the tube slanting add 4 drops of water (1 drop after another slowly). Stir well. This is called the Sodium fusion extract.		
a. EXTRACT + $FeSO_4$+50% H_2SO_4(1 drop each)	No blue or green colouration or precipitate	Absence of nitrogen
b. EXTRACT + sod. niroprusside(1 drop each)	No violet colour	Absence of halogens
c. EXTRACT + lead acetate (1 drop each)	No black ppt	Absence of sulphur

III. DETERMINING WHETHER ALIPHATIC OR AROMATIC		
1. A little of the compound is heated in a nickel spatula.	Burns with a sooty flame	Presence of aromatic compound
	Chemistry of reaction : Aromatic compound has high carbon content	
2. Nitration test: A little of the compound is added to nitrating mixture(a mixture of 1ml each of concentrated nitric acid and concentrated sulphuric acid)and boiled in a water bath for 15 minutes. The contents are poured into a beaker containing cold water	Yellow coloration	Presence of aromatic compound
	Chemistry of reaction : Nitro derivative is formed	
IV. DETERMINING WHETHER SATURATED OR UNSATURATED		
1. Baeyer's test: 2-3 drops of dilute potassium permanganate solution is added to a solution of pinch of compound in water and shaken well.	No decolourisation of permanganate solution	Compound is saturated
	Chemistry of reaction: Potassium permanganate do not react with saturated compound.	
2. Bromine water test: 2-3 drops of bromine water is added to a solution of a pinch of compound in water and shaken well.	No decolourisation of bromine water	Compound is saturated
	Chemistry of reaction: Bromine water do not react with saturated compound.	
3. Bromine water in CCl_4 test: A pinch of the compound is dissolved in carbon tetrachloride and 2-3 drops of bromine in carbon tetrachloride solution is added.	No decolourisation	Saturated compound
V. IDENTIFICATION OF FUNCTIONAL GROUP		
1. Test with sodium bicarbonate: A drop of the substance is dissolved in a drop 10% sodium bicarbonate and noted the observation.	Brisk effervescence	Presence of carboxylic acid.

	Chemistry of reaction: Carbon dioxide is formed.	
	No yellow or brown solution or smell of ammonia	Absence of carbohydrate and amide
3. The above solution is acidified with concentrated hydrochloric acid.	No white precipitate and no smell of ammonia in the above test.	Absence of amide and ester
4. Test with concentrated sulphuric acid: A small amount of the compound is heated with concentrated sulphuric acid in adry test tube.	No charring with the smell of burnt sugar and doesnot dissolve on heating.	Absence of carbohydrate and polynuclear hydrocarbon
5. Test with soda lime: A small amount of the compound is heated strongly with soda lime.	Kerosene smell	Presence of acid
	Chemistry of reaction: acid undergoes decarboxylation and hydrocarbons are formed.	
6. Test with metallic sodium: To a little of the compound dissolved in dry benzene, a piece of metallic sodium is added.	No brisk effervescence	Absence of alcohol
7. Test with neutral ferric chloride: A small amount of the compound is dissolved in alcohol and 2-3 drops of neutral ferric chloride solution is added.	Buff coloured precipitate	Presence of benzoic, phthalic or cinnamic acid.
	Chemistry of reaction: basic ferric carboxylates are formed.	
8. Test with Borsche's reagent: A small amount of the compound is mixed with 2ml of Borsche's reagent, kept in a boiling water bath for 10 minutes and dilute hydrochloric acid is added.	No yellowish orange precipitate	Absence of aldehydes and ketones
9. Molische's reagent test: To a small amount of the compound dissolved in water, 2-3 drops of alcoholic solution of alpha naphthol is added. 1ml of concentrated sulphuric acid is added along the sides of the test tube without shaking.	No violet ring	Absence of carbohydrates

VI. CONFIRMATORY TESTS		
1. Fluorescein test: Take a micro test tube by naming as Tube A with 2ml water dissolved by 2 drops of 50% NaOH. Take another test tube with name as Tube B with a pinch of substance, resorcinol and one drop of con.H_2SO_4. Heat to dissolution. A peck of it on the tip of the glassrod is introduced in to Tube A.	Green Fluorescence	Presence of dicarboxylic acid confirmed
	Chemistry of reaction: A fluorescent dye called fluorescein is formed.	
RESULT The given organic compound is aromatic, saturated dicarboxylic acid.		

Results and discussions

1) Physical chemistry experiment-

The partition coefficient of I_2 between CCl_4 and H_2O

The partition coefficient of I_2 between CCl_4 and H_2O is determined using micro scale technique and it is found to be 89.800. The time taken for the completion of this experiment is only 10 minutes.

Conducting this experiment in micro scale helps to solve the concerned problems associated with the conventional method as it uses minimum quantity of chemicals and safe equipment's like micropipettes which do not involve mouth pipetting. In addition sharp results are obtained too.

2) Inorganic qualitative mixture analysis

5 samples of inorganic mixtures containing eliminating radicals were analyzed by micro scale method. Scheme for one of the mixture sample is reported here.

3) Organic qualitative mixture analysis

The analysis and identification of unknown organic compounds constitutes a very important aspect of experimental organic chemistry. We will have a definite procedure that can be generally applied to organic qualitative analysis. The conclusion gives a result.

The three experiments are conducted using micro scale experimental techniques. In the physical chemistry experiment, sharp value of partition coefficient of I_2 between CCl_4 is obtained in a short span of time. In inorganic mixture analysis, we are able to determine both the anions and cations clearly without doing the elimination process. And organic qualitataiveanalysis, we are able to determine the organic compounds clearly. This reflects that, micro scale experimental techniques are readily feasible in three physical experiments, organic and inorganic mixture

analysis. It also hints the wide chances of micro scale experimental techniques in other streams of chemistry. With this project, it is found that, micro scale technique is an excellent alternative for the conventional method that is practiced in our schools and colleges.

Conclusion

The study of micro scale experiment by means of the above mentioned project has proven that micro scale experimental techniques are safer, cost effective, speedy, ecofriendly and sharp result yielding compared to the usually practiced laboratory techniques. Only milligram levels of chemicals are used and clear results are obtained within short span of time. As far as B. Sc. curriculum is concerned, the project reflects that micro scale experimental techniques are more student friendly as well as eco-friendly. The experimental methods employed are much simple which in turn helps to improve the practical skills of the students. In addition very small amounts of wastes are eliminated which is a solid evidence for the environment friendly nature of micro scale chemistry. Micro scale chemistry can therefore be perfectly described as a 'small scale green chemistry'.

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Food habits among women and effects on emotional behaviour

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Abstract

In today's smart world everyone has their taste for food and their own likes for the food they consume. Nobody is ready to compromise for the food they like; the options to consume our tasty food are limitless. People are able to get their best food even it is homemade or foreign. In early times the situation was that we eat whatever we get but now the situation is we eat whatever we want. So, the food habits have influenced our lifestyle in many aspects. Sensory responses to the taste, smell, and texture of foods help determine food preferences and eating habits. However, sensory responses alone do not predict food consumption. The study was conducted with the objectives to find the food habits, taste preference and emotional behaviour of sample. The samples selected were 40 Women in the age groups of 20-50 years. The sample was selected using random sampling technique from Angamaly area.Questionnaire method was adopted for data collection. The great part of women prefers 3 meals every day. Most of the women are non- vegetarian and the food habits are similar. Most women are crazy about sweet food.Major portion of women agree they are cool minded and they rarely express their feelings openly. The study says that most of the women does not express anger in public. Most of them say that the emotional behaviour is different from the past generation. Almost half of the women agree that food habits influence emotional behaviour and spicy food influence emotional behaviour. More than half of the women agree new generation spicy foods have influenced the emotional expression of the present generation.Women agree that emotions influence their eating habits. Almost half of the women agree that they eat to satisfy emotional needs.The present study can be concluded that behaviour and food pattern is closely associated. Emotions and behaviour are triggered by the foods eaten. Hence low spice quality food which is nutritious is recommended for a healthy living.

Key words

Food habits, emotional behaviour, Spicy foods.

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Introduction

Human behaviours and emotional expressions are related to their food habits. In the present world everyone is different, and their emotional behaviours differ from each other. Their food habits play a vital role in their behaviour.Emotional eating is defined as the "propensity to eat in response to positive and negative emotions." While the term emotional eating often refers to eating as a means of coping with negative emotions, it also includes eating for positive emotions such as eating foods

when celebrating an event or eating to enhance an already good mood. In these situations, emotions are still driving the eating but not in a negative way.

Taste preferences influencing food choice vary among individuals, depending on many factors such as culture, learning experiences, and genetics. The first level of information determining whether to consume or avoid a food item is transmitted via sensory stimuli. Vision, olfaction, and taste, as well as perception of temperature or texture, provide this primary information.

Sensory responses to the taste, smell, and texture of foods help determine food preferences and eating habits. However, sensory responses alone do not predict food consumption. In reality, there are multiple links between taste perceptions, taste preferences, food preferences, and food choices and the amount of food consumed. Taste responses are influenced by a range of genetic, physiological, and metabolic variables. The impact of taste factors on food intake further depends on sex and age and is modulated by obesity, eating disorders, and other pathologies of eating behaviour. Food preferences and food choices of populations are further linked to attitudinal, social, andprobably most importanteconomic variables such as income.

In today's smart world everyone has their taste of food and their own likes for the food they consume. Nobody is ready to compromise for the food they like; the options to consume our tasty food are limitless. People are able to get their best food even it is homemade or foreign.

The study entitled "Food habits among women and effects on emotional behaviour" was undertaken with the following objectives to determine food habits of sample, to study the taste preference of sample and to find out the emotional behaviour of sample

Materials and Methods

Selection of area

The area selected for the study was Angamaly in Ernakulam district. The area was selected for the convenience of investigation and the availability of enough samples.

Selection of sample

The samples selected were 40 Women in the age groups of 20-50 years. The sample was selected using random sampling technique.The questionnaire method was used for the collection of information. . The questionnaire comprised of questions related to elicit information's related to the topic. The data collected were consolidated tabulated and analysed.

Results and Discussion

The result of the study on "Food habits among women and effects on emotional behaviour" are discussed in the following tables:

Table 1. Age wise distribution of sample

Age	Frequency (n=40)	Percentage(%)
20-30	10	25
30-40	17	42.5
40-50	13	32.5

It was observed that 25% of women aged between 20-30 years, 42.5% women were in the age group of 30-40, and 32.5% women between 40-50 years.

Table 2. Number of meals a day

Type of food	Frequency (n=40)	Percentage (%)
Vegetarian	8	20
Non-Vegetarian	29	72.5
Ovo vegetarian	2	5
Lacto Vegetarian	1	2.5

In The above table 20% of women are vegetarian, 72.5% women are non-vegetarian, 5% of women are ovo-vegetarian, and 2.5% of women are lacto vegetarian.

Table 3. Taste preferred by the sample

Type of taste	Frequency (n=40)	Percentage (%)
Sweet	12	30
Spicy	11	27.5
Salt	4	10
Sour	2	5
All types	11	27.5

The above table shows 30% of women mostly prefer sweet, 27.5% women prefer spicy, 10% women prefer salt, 5% women prefer sour and 27.5 % women prefer all types.

Table 4. Favourite taste preferred by the sample

Type of taste	Frequency (n=40)	Percentage(%)
Sweet	13	32.5
Salt	2	5
Spicy	10	25
Sour	2	5
All Types	13	32.5

The above table shows that 32.5% women are crazy about sweet, 5% are crazy about salt, 25% women are crazy about spicy, 5% are crazy about sour and 32.5% are crazy about all types

Table 5. Mood of the person

Mood	Frequency (n=40)	Percentage (%)
Cool	21	52.5
Angry	19	47.5

From the above table 52.5% women are cool minded and 47.5% women are angry.

Table 6. Self-Evaluation by the sample

Behaviour	Frequency (n=40)	Percentage (%)
Cool & Calm	13	32.5
Angry & Aggressive	10	25
Rarely Aggressive	9	22.5
Spontaneous reaction	8	20

The above table shows that 32.5% women are cool & calm, 25% are angry & aggressive, 22.5% women are rarely aggressive and 20% are spontaneous reaction.

Table 7. Frequency of outward expression of emotion.

Frequency	Frequency (n=40)	Percentage (%)
Frequently	11	10
Occasionally	18	45
Rarely	18	45
Not at all	-	-

The above table reveals that 10% of women frequently express their emotions openly and 45% women occasionally or rarely express their emotions openly.

Table 8 Express Anger in society

Frequency	Frequency (n=40)	Percentage (%)
Frequently	-	-
Occasionally	4	10
Rarely	17	42.5
Not at all	19	47.5

The above table reveals that 10% women occasionally express anger in public, 42.5% rarely express their anger in public and 47.5% women does not express anger in public.

Table 9. Influence of Food habits on emotional behaviour.

Details	Frequency (n=40)	Percentage (%)
Influenced	21	52.5
Not influenced	19	47.5

The above table reveals that 52.5% women's emotional behaviour is influenced by food habits and 47.5% are not influenced.

Table 10. Emotional eating behaviour

Eating behaviour	Frequency (n=40)					
	Yes	%	No	%	Sometimes	%
Eat more when feeling stressed	1	2.5	29	72.5	10	25
Eating habits while feeling filled	2	5	24	60	14	35
Eat when feel better (calm, soothe,etc..)	7	17.5	21	52.5	12	30
Reward yourself with food	13	32.5	8	20	19	47.5
Eat regularly until stuffed yourself	6	15	17	42.5	17	42.5
Food make you feel safe	28	70	6	15	6	15
Feel like food is a friend	21	52.5	8	20	11	27.5
Food tempts you consume and loose control	4	10	16	40	20	50

Most of them feel food as friend (52.5%), while some reward themselves with food (32.5%). Most of them have of food making them safe (70.0%).52.5 percent never felt calm or soothe nor felt better with food. 42.5% never stuffed themselves with food.

Table 11. Emotional eating triggers.

Changes in emotions	Frequency (n=40)			
	Yes	%	No	%
Eating to calm down emotions	22	55	18	45
Eating due to boredom or feeling emptiness	18	45	22	55
Eating to satisfy nostalgia or childhood habits	33	82.5	7	17.5
Eating in get together though not hungry	26	65	14	35
Family or circle of friends encourages you to overeat	3	7.5	37	92.5
Stress make you eat more	3	7.5	37	92.5

The above table reveals that 55% of women agree they eat to calm down emotions, 45% does not agree. 45% women agree they eat due to boredom and 55% does not agree. 82.5%

women agree eating to satisfy nostalgia and 17.5% does not agree. 65% women agree they eat together with other people even not hungry, 35 does not agree. 7.5% agree that their family and friends encourage them to overeat,92.5% does not agree.7.5% agree that stress make them eat more, 92.5% does not agree.

Summary and Conclusion

Most women are in between the age of 30-40 years. The great part of women prefers 3 meals a day. Most of the women are non- vegetarian and the food habits are similar.

Most women are crazy about sweet food.Major portion of women agree they are cool minded and they rarely express their feelings openly. The study says that most of the women does not express anger in public. Most of them say that the emotional behaviour is different from the past generation.

Almost half of the women agree that food habits influence emotional behaviour and spicy food influence emotional behaviour. More than half of the women agree new generation spicy foods have influenced the emotional expression of the present generation. Most of the women agree that emotions influence their eating habits. Almost half of the women agree that they eat to satisfy emotional needs.

The present study can be concluded that behaviour and food pattern is closely associated. Emotions and behaviour are triggered by the foods eaten. Hence low spice quality food which is nutritious is recommended for a healthy living.

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The analysis of contents of fruits and vegetable juices

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Abstract

The main objective of this work is to analyses the contents in various fruits and vegetables. Fruits and vegetable are always a part of balanced diet. That means fruits vegetables provide our body the essential nutrients, i.e. Carbohydrates, proteins, vitamins and minerals.Here analysed the presence of starch, protein, minerals, through various tests and also determined acidity using pH paper, Litmus paper and volumetrically.

Introduction

Fruits and vegetables provide health benefits and important for the prevention of illness. The U.S. Department of Agriculture recommends filling half of your plate with fruits and vegetables at each meal. Fruits and vegetables contain a variety of nutrients including vitamins, minerals and antioxidants. Eating the recommended amount of fruits and vegetables each day can reduce the risk of chronic diseases.

Vegetables are rich in vitamin A, vitamin C, folate, fiber and potassium. Folate helps the body to form red bloods cells. It is especially for women of child bearing age to consume folate rich foods such as bell pepper, tomatoes and spinach to prevent neural tube defects in babies. Vitamin A richer foods such as sweet potatoes, carrot and butternut sqash help to keep your skin and eyes healthy and protect against diseases. The healthiest choices are fresh fruits or frozen without added sweeteners. Fruit is naturally low in fat, sodium, calories and rich in potassium, fiber, vitamin C and folate. Some high potassium fruits help to protect against heart diseases and lower cholesterol. VitaminC in foods like strawberries and Citrus helps in wound healing and keeping germs and teeth healthy.

Eating fruits can cut your risk of cardiovascular diseases, stroke and type ll diabetics and protect against various forms of cancer. The fruits and vegetables which are higher in fibers can reduce chances of developing coronary heart disease. Eating potassium rich foods such as bananas and potatoes can help to reduce blood pressure, reduce bone loss prevent developing of kidney stones.

Consuming an abundance of fruits and vegetables has many health benefits. High fiber fruits and vegetables can also reduce your risk of cancer.Complex organic as well as inorganic compounds present in fruits and vegetables can be tested by applying different chemical analysis like quantitative analysis, qualitative analysis etc…..

It can be concluded that complex organic compounds present in fruits and vegetables can be tested by extracting out its juice andthen subjected to various test for the identification of different organic compounds. To find out the different organic substances or to make a good awareness about the organic substances, knowledge about the constituents of different fruits and vegetables is compulsorily essential.

Fruits and vegetables include a diverse group of plant foods that vary greatly in content of energy and nutrients. Additionally, fruits and vegetables supply dietary fiber, and fiber intake is linked to lower incidence of cardiovascular disease and obesity. Fruits and vegetables also supply vitamins and minerals to the diet and are sources of phytochemicals that function as antioxidants, phytoestrogens, and anti-inflammatory agents and through other protective mechanisms. In this review, we describe the existing dietary guidance on intake of fruits and vegetables. We also review attempts to characterize fruits and vegetables into groups based on similar chemical structures and functions. Differences among fruits and vegetables in nutrient composition are detailed. We summarize the epidemiological and clinical studies on the health benefits of fruits and vegetables.

Diets high in fruits and vegetables are widely recommended for their health-promoting properties. Fruits and vegetables have historically held a place in dietary guidance because of their concentrations of vitamins, especially vitamins C and A; minerals, especially electrolytes; and more recently phytochemicals, especially antioxidants. Additionally, fruits and vegetables are recommended as a source of dietary fiber.

Most countries have dietary recommendations that include fruits and vegetables. Although dietary recommendations have many similarities, different countries choose different strategies to separate fruits and vegetables into groups. Orange fruits and vegetables are often high in carotenoids and are placed in a separate category. Yet many dark green vegetables (i.e., spinach) are also high in carotenoids. Dividing fruit and vegetables into color categories makes sense for menu planning but does not correspond with nutrient content.

Benefits of Vegetable Juice

Many of the most notable benefits of vegetable juice include its ability to improve nutrient uptake, protect the heart, increase hydration, prevent hair loses, detoxify the body, lower your risk of chronic disease, support skin health, increase circulation and strengthen the immune system, among others.

Lower chronic diseases

There is a significant amount of antioxidants found in many vegetables, including beta-carotene, lycopene, phytonutrients and phenolic compounds. This protects our body from free radicals, which include mutating healthy cells into cancerous ones. Regular consumption of vegetable juice lowers the risk of many other chronic diseases as well, including diabetics, cardiovascular disease and even some autoimmune diseases

There is a notable amount of potassium in many different juices, which can help to lower the blood pressure and relieve strain on the cardiovascular system. Furthermore, there are high quantities of iron and vitamin C, which can stimulate proper circulation and improve the amount of collagen in the body, respectively, helping to lower the risk of damaged blood vessels or arteries.

Materials and methods

Experimental methods

Here determined the acidity, presence of starch, proteins, minerals like Ca, K, Mg, Fe etc… of various fruit as well as vegetable juices. The method we adopted is the qualitative and quantitative analysis. The

acidity was determined by using pH papers, litmus papers and by volumetric analysis.

1 Test for acidity

1.2 procedure

1. 5 ml of various fruit juice were taken in different test tubes and dipped the PH paper in them. Marked the test tubes as A, B, C, D etc. so as to identify the samples.

2 Determined the acidic nature with the help of litmus paper also. Observations were recorded in tabular form.

3 10 ml of well filtered juice marked A was taken in a conical flask and diluted it to 40 ml using distilled water from the burette using phenolphthalein indicator. From the volume of 0.5N oxalic acid reacting with 20ml NaOH solution normality of NaOH solution was calculated.. Standard solution of (0.5N) sodium hydroxide is prepared and filled it in the burette. The juice in conical flask titrated against sodium hydroxide solution using phenolphthalein as the indicator .The strength of acid present in the juice was calculated. The experiment was repeated with other juices and observations were tabulated.

Standard solution of oxalic acid was prepared by weighing out about 3.15g oxalic acid using a chemical balance. It is transferred into 100 ml standard flask, add water, made up to the mark and shaken well. This is 0.5N Oxalic acid. Pipetted out 20 ml of NaOH solution into a conical flask and titrated against oxalic acid from the burette using phenolphthalein as indicator. From the volume of 0.5N oxalic acid reacting with 20 ml NaOH solution was calculated.

2. Test for starch, proteins& carbohydrates

Test for starch

3 ml of the fruit juice was taken in a test tube and a few drops of iodine solution were added in to it. Formation of a blue coloration indicated the presence of starch. The experiment was repeated with other samples.

Test for proteins

Biuret test:-To about 3 ml of NaOH solution, two drops of 1% copper sulphate solution wasadded till a permanent blue color is obtained. 2ml of the juice was added in to it and shaked well. A violet coloration (or precipitate) indicated the presence of proteins in the juice. The experiment was repeated with other samples.

Test for carbohydrates

Molisch's test: 1%solution of alpha naphthol in ethyl alcohol wasprepared. 2ml of this solution was added to 2ml of the juice taken in a test tube. Con: H2SO4was added along the sides of the test tube slowly. A violet coloration at the junction of the two layers indicated the presence of carbohydrates in the juice .The experiment was repeated with other samples.

3. Test for minerals

Test for iron

2 ml of fruit juice was mixed with two drops of Con: HNO3 and the mixture was heated. The mixture was cooled and three drops of ammonium thiocyanate (NH_4CNS) solution were added.Formation of blood red color indicated the presence of Iron. The test was repeated with other samples.

Test for phosphorous

2 ml of the juice was taken with two drops of Con: HNO_3 and the mixture was boiled. A few drops of Ammonium molybdate reagent were added in to this mixture and

heated again. Bright yellow precipitate was formedindicated presence of phosphorous in the juice. The test was repeated with other sample

Test for sodium and potassium

a) Two pellets of solid KOH were taken in to 2 ml of juice and boiled. To the hot mixture, potassium pyroantimonate solution was added and the sides of the test tube were scratched with glass rod. Awhite precipitate was formed shows the presence of sodium ions. The test was repeated with other sample.

b) 2 ml of picric acid solution was taken to 2 ml of the juice. Yellow precipitate showed the presence of potassium ions. The test was repeated with other samples.

Test for calcium and magnesium

a) 2 ml of the juice was taken with a little of solid NH_4Cl and NH_4OH solution. It was shaked well and filtered. To the filtrate add 2 ml of ammonium oxalate solutionwas added. Formation of white precipitate indicated presence of calcium ions. The test is repeated with other samples.

b) 2 ml of the juice was taken with a little of solid NH_4Cl, NH_4OH and Disodium hydrogen phosphate solution. Thesides of the test tube were scratched with a glass rod. White precipitate is presence of magnesium ion. The test was repeated with other samples.

Result and discussion

B Estimation of strength of acids

Normality of NaOH=0.485N

Sl no	JUICE	Volume of NaoH V_1 (ml)	Volume of juice taken (ml) V_2	Normality of acid in the juice $0.485*V_1/V_2$
1	LEMON	22.9	10	1.1100N
2	GRAPES	9	10	0.0436 N
3	PINEAPPLE	3.3	10	0.1600 N
4	ORANGE	3	10	0.1455 N
5	CARROT	1.2	10	0.0582N
6	TOMATO	1.1	10	0.0533 N
7	PAPAYA	1.1	10	0.0533 N
8	CUCUMBER	0.6	10	0.0291 N

SL NO	SAMPLE	ACID STRENGTH	pH	CHANGE IN BLUE LITMUS
FRUIT JUICE				
1	PINEAPPLE	0.1600 N	5	RED
2	ORANGE	0.1455N	5	RED
3	LEMON	1.110N	5	RED
4	GRAPE	0.0436N	5	RED
5	PAPAYA	0.0522N	5	RED
VEGETABLE JUICE				
6	CUCUMBER	0.0291 N	6.5	RED
7	CARROT	0.0582N	6.5	RED
8	TOMATO	0.0533 N	6	RED

TEST FOR COMPONENTS

SL.NO.	SAMPLES	STARCH (TEST WITH IODINE)	PROTEIN (BIURET TEST)	CARBOHYDRATE (MOLISCHE'S TEST)
FRUIT JUICE				
1	PINEAPPLE	Blue colour	Violet colour	Violet colour
2	ORANGE	No bluecolour	Violet colour	Violet colour
3	LEMON	No blue colour	Violet colour	Violet colour
4	GRAPE	Blue colour	Violet colour	Violet colour
5	PAPAYA	No blue colour	Violet colour	Violet colour
VEGETABLE JUICE				
6	CUCUMBER	Blue colour	Violet colour	No Violet colour
7	CARROT	blue colour	Violet colour	Violet colour
8	TOMATO	No blue colour	Violet colour	No Violet colour

SL.NO.	SAMPLE	IRON	PHOSPHOROUS	CALCIUM	MAGNESIUM
FRUIT JUICE					
1	PINEAPPLE	Blood red colour	Yellow ppt	White ppt	White ppt
2	ORANGE	Blood red colour	Yellow ppt	White ppt	White ppt
3	LEMON	Blood red colour	Yellow ppt	White ppt	White ppt

4	GRAPE	Blood red colour	Yellow ppt	White ppt	No White ppt
5	PAPAYA	Blood red colour	Yellow ppt	White ppt	No White ppt
VEGETABLE JUICE					
6	CUCUM-BER	Blood red colour	No Yellow ppt	White ppt	White ppt
7	CARROT	Blood red colour	Yellow ppt	White ppt	No Whiteppt
8	TOMATO	Blood red colour	Yellow ppt	White ppt	No Whiteppt

SL.NO.	SAMPLE	SODIUM	POTASSIUM
FRUIT JUICE (Colour of precipitate)			
1	PINEAPPLE	White	Yellow
2	ORANGE	White	Yellow
3	LEMON	White	Yellow
4	GRAPE	White	No Yellow
5	PAPAYA	White	No Yellow
Vegetable Juice (Colour of precipitate)			
6	CUCUMBER	White	Yellow
7	CARROT	White	Yellow
8	TOMATO	White	Yellow

- Fruits and vegetables juices used for analysis are acidic due to the presence of Malic acid, Tartaric acid, citric acid etc. of fruits and vegetables are different due to the variation in the amount of acid content in it.
- Blue litmus paper dipped in fruits and vegetables juices used for the analysis turns to red color. This shows that all the samples used for the analysis are acidic in nature.
- Pineapple, Grape, Carrot, Cucumber give positive result in test for starch. The others do not give positive result for the test of starch. It may because starch present in samples is not detection level.
- All samples gave positive result for protein with 5% NaOH solution. The sample show violet coloration with the reagent. Hence all fruits and vegetables juice used are rich in protein.
- All the samples gave positive result (other than tomato and cucumber) for carbohydrate. The sample gave a violet ring in Moliche's test. Hence all the fruit and vegetables used for analysis contain carbohydrate.
- All the samples tested gave positive re-

sult for iron. Samples gave blood red coloration with HNO3and potassium thiocyanate. Hence all fruits and vegetables used for analysis contain iron.

- The entire sample tested gave positive result for phosphorous other than cucumber all Samples gave yellow precipitate.
- All the samples give positive result for sodium. Samples gave white precipitate with reagents.
- All the samples give positive result for potassium. Samples gave yellow precipitate with picric acid. The juices used for analysis contain potassium.
- Papaya, Grape, Carrot, and tomato do not give positive result in test for magnesium. It may because magnesium present in samples is not detection level. The others give positive result for the test of magnesium.

Conclusion

This project gives an overall idea about the components present in both fruit juice and vegetable juices. We found the acidity, presence of starch, protein and minerals by adopting different qualitative and quantitative methods.

By the experiments we concluded that the pH range of fruits and vegetables are 3-6.5. Lemon and orange juices have the highest acid strength. All the other fruits and vegetables contain less acid content. This acid content present in juices are found by quantitatively. Hence we can found out it accurately.

All the fruits and vegetables under study contain minerals, carbohydrates and starch in different quantities and these are main sources of vitamin, minerals and dietary.

From these we could recognize the important of fruits and vegetables in our diet. It is very helpful to know which fruit or vegetables are richer in the case of nutrient content and also it gives a clear idea about the contents present in vegetables and fruits.

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Preparation and character study of cuprammonium rayon thread

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Abstract

Modern textile blends continue to require the aesthetics and moisture-absorbing properties provided by cellulose in the native state as cotton or in regenerated form. Rayon is a regenerated synthetic fiber produced from cellulose. The work is aimed to synthesize Cuprammonium Rayon Threads from filter paper and study its characteristics. Cuprammonium rayon is produced by dissolving cellulose in a deep blue solution of tetra-ammine cupric hydroxide. The structure was investigated by infrared spectroscopy the spectrum gave the confirmation of the formation of Cuprammonium rayon and its characteristics were studied by different chemical reactions.

Introduction

Fibers are typically semi crystalline polymers that can be spun into long strands that have high strength to weight ratios for textile as well as composite application. Fibers are commonly used for the manufacture of other materials .There are two types of fibers; Natural and Synthetic fibers.

Natural fibers are fibers that are produced by plants, animals, and geological processes. It is used for textile applications long before the first polymer synthesized in the laboratory. Synthetic fibers are fibers made by humans with chemical synthesis, as opposed to natural fibers that humans get from living organisms with little or no chemical changes. They are resulted from the hard work of researchers to improve on naturally occurring animal fibers and plant fibers. In general, synthetic fibers are created by extruding fiber-forming materials through spinnerets into air and water, forming a thread. These fibers are called synthetic or artificial fibers. Synthetic fibers are generally semi crystalline polymers that are capable of being spun in to filament of length to diameter ratios in excess of 100. Synthetic fibers are Rayon, Saran, and Spandex etc.

Textile yarns of synthetic polymers are produced by twisting several continuous fibers together to form a uniform structure with all filaments aligned parallel to the yarn axis. Before synthetic fibers were developed artificially manufactured fibers were made from polymers obtained from petrochemicals. Some of the fibers made from plant cellulose. They are called “cellulose fibers”.

Synthetic fibers are more durable than natural rubbers. In addition, many synthetic fibers offer consumer-friendly functions such as stretching, waterproofing and stain resistance. Sunlight, moisture, and oils from human skin cause all fibers to break down and wear away. Natural fibers tend to be much more sensitive than synthetic blends. This is mainly because natural products are biodegradable. Natural fibers are susceptible to larval insect infestation; synthetic fibers are not a good food source for fabric-damaging insects. As an advantage, synthetic fibers

do not break down easily when exposed to light, water or oil.

Compared to natural fibers, many synthetic fibers are more water resistant and stain resistant. Some are even specially enhanced to withstand damage from water or stains. Some fabrics are also designed to stretch in specific ways, which makes them more comfortable to wear. In many cases, synthetic fibers are environmental fabric choice.

Common types of Synthetic Fibers and their Properties

Synthetic fibers are used for making clothes and many other useful things. They may be entirely synthetic or semisynthetic. Semi synthetic fibers, like rayon, are made by using natural polymers as the starting material. Purely synthetic fibers, on the other hand, are made from chemicals. Polyesters, nylons and acrylics are purely synthetic fibers.

Rayon:

These are the most widely used semi synthetic fibers. Rayon is created by the regeneration of natural materials. It is made from wood pulp and its properties are similar to those of linen or cotton. There are various types of rayon including regular, high tenacity, high wet modulus and microfibers. High tenacity rayon is strong and used mainly in industry. Regular rayon is often used in clothing. High wet modulus has high wet strength and microfibers are fine and silky.

Acetate rayon:

In this case, cellulose is dissolved in a mixture of acetic acid, sulphuric acid and some other chemicals. The solution is forced through spinnerets to obtain filaments of acetate rayon. Acetate rayon is soft and silky and drapes well. Acetate is also used to make home furnishings such as drapes and bedspreads. Acetate is resistant to mildew and shrinkage and is often used to make linings because it absorbs moisture from the body

Acrylic:

Synthetic textile is acrylic which is soft and luxurious and also drapes well. It is not a heavy fabric but it gives warmth. It was originally used to make outdoor goods but now is common in clothing and carpet although pure acrylic can result in pilling. Acrylic is made from a petrochemical called acrylontrile.

Polyester:

Polyester is soft and strong, resistant to shrinkage and does not stretch. It is a polymer which is produced from coal, water, air and petroleum products. It can blend with natural fibers such as cotton or wool or with artificial ones, to increase the fabric more durable and easier to wash. It can be used in clothing, filling for upholstery, floor coverings and insulation.

Nylon:

Nylon is a polymide which is made from petroleum. It was discovered by a chemist named Du Pont. It is durable and lightweight. Nylon is quick drying and cleans easily because dirt does not cling. It can be static and does not absorb moisture so, if used it clothing, it can be clammy in the heat. Examples of nylon products include luggage, carpeting materials and hosiery because of its elastic recovery ability.

Rayon

Artificial silk or Rayon is one of the most important commercially use synthetic fibers of the modern era. Although this fiber was discovered in the 17th century, it becomes prominent in the textile world for the first time in France in 1890.

Artificial silk is a man-made or arti-

ficial fiber whose chemical base is the cellulose; it can be prepared from cellulose.

Nitrocellulose rayon: It is manufactured from colloidion cotton. The cotton is obtained by the coagulation of cotton in colloidal solution. The colloidon cotton is dissolved in a mixture of alcohol (1 vol) and ether (3 vols) to form a colloidal solution of colloidon.

Cuprammonium rayon: The cuprammonium rayon yarn is manufactured from filaments obtained by the coagulation of a solution of cellulose in an ammoniacal solution of copper hydroxide called schweizter's reagent. The cupric hydroxide is obtained by treating copper sulphate with sodium hydroxide.

Acetate rayon: It involves convertion of cellulose into a solvent soluble acetyl derivative permitting formation of fiber and removal of solvents by evaporation. It is soft and provides warm feelings, it is used for all kinds of men and women wears such as ties, shirts, pajamas, dressing gowns, shocks, etc. It is also used as insulator for electric wirings and coils. Due to low hydroscopicity it is not suitable for making handkerchiefs and fabrics subjected to hard wear0 due to its moderate resistance to abrasion.

Viscose rayon: The silky threads thus obtained are spun on a bobbin, desuphurised, washed with soap solution, twisted to form yarn, bleached with NaOCl and dried. This silk is known as viscose rayon.Vicose fibers are widely used in making dress linings, curtains, table cloths, bed covers, fine fabrics, cushions, sports wears etc.

Cuprammonium Rayon

Cuprammonium Rayon is made from cellulose dissolved in cuprammonium solution. It is produced by making cellulose a soluble compound by combining it with copper and ammonia. The solution of this material in caustic soda is passed through the spinneret and the cellulose is regenerated in the hardening baths that remove the copper and ammonia and neutralize the caustic soda. Cupro is usually a very light, fine, soft, fabric, and is used as linings in quality suits and dresses, as it tends to last better than silk, but is nicer to feel and wear than acetate.

Cuprammonium rayon is made by dissolving cellulose in an ammoniacal copper sulphate solution. This when diluted with water or treated with dilute Sulphuric acid solution, the cellulose is regenerated or re-precipitated. By using a spinneret, filaments of this regenerated cellulose can be produced, as in the case of viscose rayon. Cuprammonium rayon has properties similar to viscose but during production, the cellulose is combined with copper and ammonia.

Chemical nature of cuprammonium process

Ammonical copper oxide solution is also known as cuprammonium hydroxide solution. Cuprammonium hydroxide solution is a solvent for cellulose. When a solution of cellulose in cuprammonium hydroxide is diluted with water or treated with dilute sulphuric acid, the cellulose is regenerated or reprecipitated. By using a spinnerette, filaments of this regenerated cellulose can be produced. The basis of the manufacture of cuprammonium rayon is the solubility of cellulose in an ammoniacal copper oxide solution. If cellulose is treated with this solution, the hydrogen bonds forming capacity of the hydroxyl groups of cellulose in the amorphous region is destroyed and the hydrogen bonds present in the crystalline region are broken and these hydroxyl groups are also fixed. As a result, cellulose dissolves.

The reactions involved are as follows:

$2NH_4OH(aq) + CuSO_4(aq) \rightarrow Cu(OH)_2(s) + (NH_4)_2SO_4(aq)$

$Cu(OH)_2(aq) \rightarrow Cu^{2+}(aq) + 2OH^-(aq)$

$n\ Cu^{2+}(aq) + (cellulose)\ n + 2n\ OH^- \rightarrow (CuC_6H_8O_5)\ n + 2n\ H_2O$

Preparation of rayon by cuprammoniumprocess

The Cuprammonium rayon is manufactured from filaments obtained by coagulation of a solution of cellulose in an ammoniacal solution of copper hydroxide, $Cu[(NH_3)_4](OH)_2$, called Schweitzer's reagent. The process is based on the observation that cellulose soluble in ammoniacal copper oxide and can be regenerated from solution by adding acid.

$2NH4OH + CuSO_4 \rightarrow (NH_4)_2SO_4 + Cu(OH)_2$

$(NH_4)_2SO_4 + Cu(OH)_2 \rightarrow Cu(NH_3)_4(OH)_2$

It is regenerated from the solution by adding Sulphuric acid. Thus rayon regenerated cellulose and it is used for making fabrics like stockings, shirts etc. The cuprammonium rayon can be also prepared by using NaOH and wood pulp.

Manufacture of wood pulp:

Wood pulp is produced by the sulphite process. Chips of wood are digested in a digester with aqueous solution of calcium bisulphite and with excess of sulphurous acid at in temperature of 130^0 to 145^{0C} and a pressure of 70 to 100 psi for 7 to 12 hours. After the digestion, the pulp formed is washed with water, bleached and pressed into sheets.

Manufacture of cotton pulp:

Cotton linters are attached to the cotton seed. The linters are digested with 3 per cent caustic soda solution at above 60psi for four hours. After this period the pump pulp is washed with water, bleached and formed into sheets. The cotton pulp contains 98% of alpha cellulose while the wood pulp containing 88-98% alpha cellulose.

Preparation of cuprammonium rayon:

The wood pulp or cotton linter pulp is taken in a mixture filled with a stirrer and concentrated to vaccum. The pulp is dissolved by adding Schweitzer's reagent with constant stirring. The excess of ammonia in the solution is withdrawn from the mixture through vaccum line. The cellulose is dissolved by stirring and the resultant solution is filtered several times. The filtrate is forced through the orifices of the spinnerets into a stream of water which stretched the filaments and this are then passed through a 1.5 per cent solution of Sulphuric acid. The later destroys the cuprammonium complex and precipitate cellulose. The filaments are thoroughly washed to remove all soluble substance, bleached, dried and passed round the pulley and finally got round on the bobbin. These filaments are better than silk fibers.

Materials and methods

Chemicals required

- $CuSO_4$
- NaOH solution
- Liquor ammonia solution
- Dilute H_2SO_4
- Distilled H_2O

Procedure

Preparation of Schweitzer's Solution:

a. Weigh 20g of $CuSO_4 5H_2O$.

b. Transfer this to a beaker having 100 ml distilled water and add 15 ml of dilute H_2SO_4 to prevent hydrolysis of $CuSO_4$.

c. Stir it with a glass rod till a clear solution is obtained. Add 11ml liquor ammonia drop by drop with slow stirring. The precipitate of cupric hydroxide is separated out.

d. Filter the solution containing cupric hydroxide through a funnel with filter paper.

e. Wash the precipitate of cupric hydroxide with water until the filtrate fails to give a positive test for sulphate ions with barium chloride solution.

f. Transfer the precipitate to a beaker that contains 50 ml of liquor ammonia or wash it down the funnel. The precipitate when dissolved in liquor ammonia gives a deep blue solution of tetra-ammine cupric hydroxide. This is known as SCHWEITZER'S SOLUTION.

Preparation of Cellulose material:

a. After weighing 2g of filter paper divide it into very fine pieces and then transfer these pieces to the tetra-ammine cupric hydroxide solution in the beaker.

b. Seal the flask and keep for 10 to 15 days, during this period the filter paper is dissolved completely.

Formation of Rayon Thread:

a. The 50mlof distilled water in a glass container .To this adds 20ml of con. H2SO4 drop by drop .Cool the solution under the tap water. In a big glass container pour some of the solution.

b. Fill the syringe with cellulose solution prepared before.

c. Place the big glass container containing H_2SO_4 solution produced before in ice (the reaction being spontaneous result in excess release of energy in the form of heat which makes the fibers weak and breaks them).

d. Immerse the tip of the syringe in the solution and press gently .Notice the fibers getting formed in the acid bath. Continue to move your hand and keep pressing the syringe to extrude more fibers in to the bath.

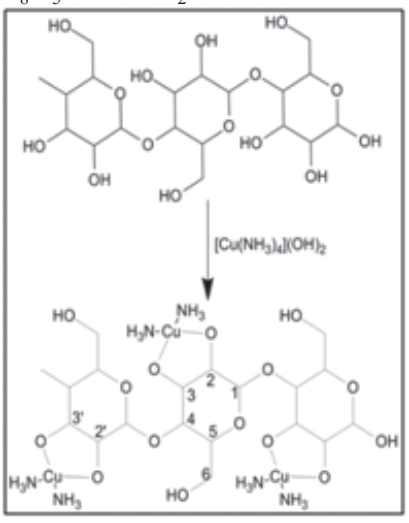
e. Leave the fibers in solution till they decolorize and become strong enough.

f. Filter and wash with distilled water (Plate I)

$2NH_4OH\ (aq) + CuSO_4(aq) \rightarrow Cu(OH)_2\ (s) + (NH_4)_2SO_4(aq)$

$Cu\ (OH)_2\ (aq) \rightarrow Cu^{2+}(aq) + 2OH^-\ (aq)$

$n\ Cu^{2+}(aq) + (cellulose)n + 2nOH^- \rightarrow (CuC_6H_8O_5)n + 2nH_2O$



Steps involved in Rayon thread formation

Fig.1
Preparation of Schweitzer's Solution from Copper sulphate and ammonia solution

Fig.2.
Schweitzer's Solution

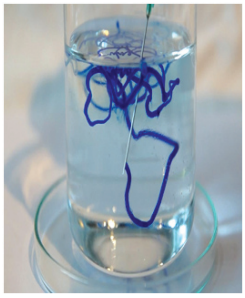


Fig. 3.
The introduction of cellulosic solution into Sulphuric acid bath

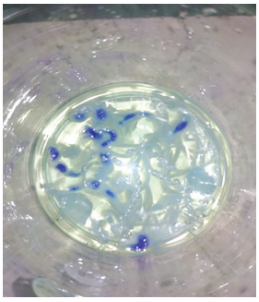


Fig. 4.
Rayon Thread

Result and Discussion

Cuprammonium rayon thread is prepared by cuprammonium process. The method is based on the fact that cellulose dissolves in ammoniacal copper oxide and can be regenerated by adding acid. It is done in three stages. First, preparation of cuprammonium hydroxide or Schweitzer's solution – A definite amount of copper sulphate is treated with a known volume of ammonia solution. The precipitate formed is filtered, washed thoroughly and then excess ammonia solution is added. Second, preparation of cellulosic material – small pieces of filter paper is added to the Schweitzer's solution and kept as such for 10-15 days. Filter paper completely dissolves in the solution. Third, production of rayon thread – The cellulosic solution is then introduced into the sulphuric acid bath with a syringe. The rayon threads are formed.

A few important properties of Cuprammonium rayon are studied:

Appearance: Cuprammonium rayon resembles like glass rod and cross section is round

Action of heat: A small quantity of Cuprammonium rayon is burned in a spatula. It burns like cotton and get charred, with the smell of burning of cotton.

Cuprammonium rayon resembles cotton in character and burns like cotton.

Solubility: a) In Acid: One or two gram of Cuprammonium rayon is taken in a test-tube. A little conc. HCl (or con.H_2SO_4) is added and shaken well. It dissolves.

Cuprammonium rayon is soluble in strong acid.

b) In Alkali: One or two gram of prepared cuprammonium rayon is introduced into a test tube containing NaoH and shaken well. It is only partially soluble.

Cuprammonium rayon thread is sparingly soluble in alkali.

Action of sunlight and air: Small pieces of rayon thread are kept in light. It is noted that, rayon is degrading slowly and its water content is increasing progressively in presence of light.

Cuprammonium rayon is degraded and weakened by exposure to sunlight in the presence of air and moisture.

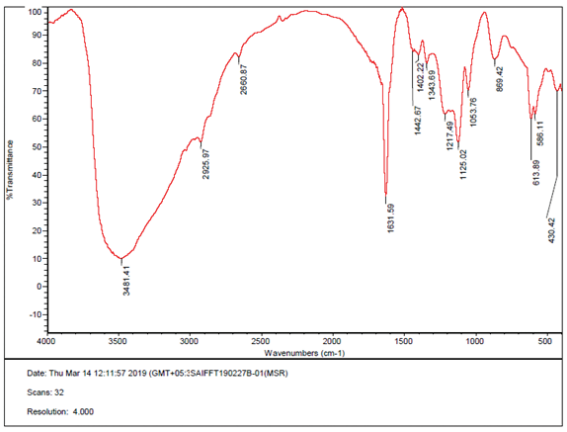


Fig. 5. IR Spectrum of Cuprammonium Rayon

Figure shows the infrared spectra of Cuprammonium rayon in the region of 4000-500 cm^{-1}. 1053 cm^{-1} and 1125 cm^{-1} corresponds to the C-O-C asymmetric stretching, 1343 cm^{-1} corresponds to CH_2 in plane bending vibration in cellulose. The peak at 1631 cm^{-1} may be attributed to the HOH bending of absorbed water. The broad peak at 3481 cm^{-1} corresponds to O-H stretching vibration of Cellulose.

Conclusion

Synthetic fibers account for about half of all fiber usage, with applications in every field of fiber and textile technology. A great advantage of synthetic fiber is that they are more durable than most natural fibers. One of the common types of synthetic fiber is rayon. It is a regenerated fiber, because cellulose is converted to a liquid compound and then back to cellulose in the form of fiber. Cuprammonium rayon is simply cellulose dissolved in a cuprammonium solution. It is obtained by dissolving pieces of filter paper in a deep blue solution containing tetra-ammine cupric hydroxide.

Cuprammonium rayon thread resembles cotton in character. It appears like glass rod and cross section is round. It is known that the dye absorption power for direct dyes of cuprammonium rayon is greater and shades obtained are deeper than viscose rayon, other conditions of dying being kept constant. Extreme fineness, smooth a soft nature makes it a versatile fiber. The infrared spectra of Cuprammonium rayon in the region of 4000-500 cm^{-1} clearly imply the structure of cellulose in cuprammonium solution.

This project work has helped us to understand the importance of synthetic fibers, rayon thread is prepared by a simple process and its characteristics are also studied.

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Calculations of pKa values of some organic compounds using computational chemistry calculations

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Abstract

The pKa of anorganic compound is one of its most important properties as it defines the specific molecular forms that will prevail under different pH conditions. Finding a theoretical calculation method to obtain the accurate solvation free energy and pKa value so as to verify or complement the experimental data has long been an important aspect in recent years. We have modeled simple gaseous phase deprotonation reactions and calculated the pKa of various organic molecules such as Trifluoromethane, Ethylene, Phenol, cyclopropane, methane and ethanol,Benzoic acid etcusing HF/6-31G method. We also compare the results with the experimental data and found that for electron rich species and carboxylic acid the results are in good agreement with the experimental data.

Introduction

The field of computational chemistry has become an extremely valuable research tool in chemistry, physics, and biology. Computational chemistry began with quantum theory, which is the study of the interaction of atoms with each other and with energy at the subatomic and atomic level. Quantum theory aims to predict the behavior of atoms based on the physics principles that apply at such a small scale. Calculations using quantum mechanics-based equations such as the wave function and Schrödinger equation allow scientists to analyze and predict various characteristics and behaviors of both atoms and molecules. Before computers, this work was very cumbersome and nearly impossible to complete. With the improvement of computer technology, computational chemistry programs were developed and provided an immeasurably easier way to perform these necessary calculations. With this type of computer software, the user gives the computer input of some molecular properties. Based on the software and the given input, the program will perform calculations to model various characteristics of the given molecule, such as geometry, energy, and intermolecular forces. Both chemists and biochemists benefit from the ability of computational software to simulate reactions, particularly those involving substances dangerous to work with or difficult to obtain.

The computer programs are based on quantum mechanics, classical mechanics and statistical mechanics. The development of computational chemistry and its application to existing chemical problems had led to better advancement in the field of chemistry within a short time. The main advantage of computational chemistry is that better result can be obtained in a short period of time which may take long time when done manually.

The areas in which the computation chemistry finds application are molecular geometry calculations, to predict energies of molecular and transition state, chemical reactivity, IR, UV and NMR spectra and interaction of substrate with enzyme. The important application of computational chemistry is in the field of drug design about 10 drugs developed using this technique is now used in the medical treatment. pKa is negative logarithm of base 10 of acid dissociation constant Ka. pKa = -logKa The pKa values have wide application in chemistry and bio molecular processes in living organism. In thermodynamic study of mechanism of enzyme catalysis acid dissociation constant is used. The use of acid dissociation constant in enzymatic catalysis makes the calculation convenient to take base 10 logarithms of equation. Acid dissociation constant and dissociation constant determine the concentrations of species present in a solution at equilibrium under specified conditions1. It has been widely used in drug discovery process. The pKa values of a deprotanation reaction can be calculated from Gibbs free energy of reaction. In our project we are calculating the pKa values of some organic compound using Gaussian software. Method used to calculate Gibbs free energy of deprotonation reaction is Hartree-Fock method and basis set 6-31G and thereby calculate pKa value. And also we are comparing the theoretically calculated pKa values using experimentally calculated pKa values.

Tools of Computational chemistry

Computational chemistry is based on theoretical calculation of chemical properties of molecules. The basic tools used in computational chemistry calculations are of five broad classes.

Molecular mechanics (MM)

It based on model of molecule as a collection of balls held together by springs. The balls represent the atoms and springs represent bonds in the molecule. By knowing the normal bond lengths and bond angles of the molecule and how much energy is needed to stretch and bend bond one can calculate the energy of given molecule. Thus we can calculate the geometry for molecule. Using this geometry of steroids can be optimized in few seconds.

Ab initio calculations

It is based on the Schrodinger equation. Ab initio method solves Schrodinger equation for a molecule and gives us molecule's energy and wave functions [2]. Wave function is a mathematical function that can be used to calculate the electron distribution2. From electron distribution we can understand the polar nature of molecule and the electrophilic and nucleophilic sites of molecule. Semiempirical (SE) calculations It also based on Schrodinger equation but parameterized with experimental values 2.

Density functional theory (DFT)

Like ab initio and SE calculation it is based on Schrodinger equation. Unlike other two methods DFT directly derives electron distribution without calculating wave function. Molecular dynamics calculations It applies laws of motion to molecules. Thus one can stimulate the motion of an enzyme as it changes shape on binding to a substrate2. It studies about molecules in motion.

HartreeFock method

HartreeFock method is aab initio method. Ab initio is a Latin word with meaning from the beginning. It is most common type of ab initio calculation in which the principle approximation is the central field approximation. This means that the Coulombic electron-electron repulsion is taken into account by integrating the repulsion term. This gives the average effect of repulsion, but not the explicit repulsion interaction. This is a variational calculation, meaning that the approximate energies calculated are all equal to or greater than the exact energy. The energies are calculated in units called Hartrees(1 Hartree = 27.2116 eV). Because of central field approximation, the energies from HF calculations are always greater than the exact energy and tend to a limiting value called Hartree-Fock limit as the basis set is improved3. One of the advantages of this method is that it breaks many electrons Schrodinger equation in too many simpler one electron equations. Each one electron equation is solved to yield a single electron wave function, called an orbital, and an energy called orbital energy. The orbital describe the behavior of electron in the net field of all other electrons3. The second approximation in HF calculation is due to the fact that the wave function must be described by some mathematical function, which is known exactly for only a few one – electron systems. The functions used most often are linear combinations of Gaussian-type orbitals abbreviated as GTO. The wave fuction is formed from linear combination of atomic orbital or from linear combination basis functions. Because of this approximation, most HF calculation gives a computed energy greater than the Hartree-Fock limit. The exact set of basis functions used is often specified by an abbreviation STO-3G3.

Basis set

A basis set is a set of functions used to describe the shape of the orbitals in an atom. Molecular orbitals and entire wave functions are created by taking linear combinations of basis functions and angular functions. Most semiemperical methods use a predefined basis set. When ab initio or density functional theory calculations are done, a basis set must be specified. The type of calculation performed and basis set chosen are the two biggest factors determining the accuracy of results3. The smallest basis sets are called minimal basis sets. The most popular minimal basis set is the STO-3G set. This notation indicates that the basis set approximates the shape of a STO orbital by using a single contraction of three GTO orbitals. One such contraction would then be used for each orbital, which is the definition of a minimal basis. Minimal basis sets are used for very large molecules, qualitative results, and in certain cases quantitative results. There are STO-nG basis sets for n = 2-6. [3] Another family of basis sets, commonly referred to as the Pople basis sets, are indicated by the notation 6-31G. This notation means that each core orbital is described by a single contraction of six GTO primitives and each valence shell orbital is described by two contractions, one with three primitives and the other with one primitive. These basis sets are

very popular, particularly for organic molecules. Other Pople basis sets in this set are 3-21G, 4-31G, 4-22G, 6-21G, 6-311G, and 7-41G. [3] STO-nG (n = 2-6) n primitives per shell per occupied angular momentum …(s, p, d). STO-3G is heavily used for large systems and qualitative results. The STO-3G functions have been made for H with three primitives (3s) through Xe(15s12p6d). STO-2G is seldom used due to the poor quality of its results. The larger STO-nG sets are seldom used because they have too little flexibility. [3] 6-31G Available for H(4s) through Ar(16s10p). Very popular for quantitative results for organic molecules.[3] Both Slater Type Orbitals (STOs) and Gaussian Type Orbitals (GTOs) are used to describe AOs. STOs describe the shape of AOs more closely than GTOs, but GTOs have an unbeatable advantage: they are much easier to compute. In fact, it is faster to compute several GTOs and combine them to describe an orbital than to compute one STO! This is why combinations of GTOs are commonly used to describe STOs, which in turn, describe AOs. Gaussian theory

The Gaussian methods (G1, G2, and G3) are also unique types of computations. These methods arose from the observation that certain ab initio methods tend to show a systematic error for predicting the energies of the ground states of organic molecules. This observation resulted in a correction equation that uses the energies of several different ab initio calculations in order to extrapolate to a very high accurate result. All the calculation that goes in to this extrapolation are ab initio methods. However, the extrapolation equation itself is an empirically defined equation parameterized to reproduce result from a test set of molecules as accurately as possible. The extrapolation to complete correlation is based the number of electrons times an empirically determined constant. For this reason, these methods show same strength and weakness as other semiemprircal methods. The accuracy can be extremely good for systems similar those for which they were parameterized, he ground state of organic molecules. However this methods are less accurate for other systems such as transition structure or clusters than some less computationally intensive ab initio methods3.

Thermo-chemical calculations using Gaussian software

In this section, we outline the various computational steps adopted in the Gaussian software[11, 12] to obtain Gibbs free energy of various gaseous phase reactions.All frequency calculations include thermochemical analysis of the system. By default, this analysis is carried out at 298.15 K and 1 atmosphere of pressure, using the principal isotope for each element type. Gaussian predicts various important thermodynamic quantities at the specified temperature and pressure, including the thermal energy correction, heat capacity and entropy. It also give the zero point energy (ZPE). These items are broken down into their source components in the output. Here we present a sample output of thermochemical data obtained from the combined optimization and frequency calculations.

```
Zero-point correction=                          0.029209 (Hartree/Particle)
Thermal correction to Energy=                   0.032062 (Etherm = ZPE+Etrans+Erot+Evib)
Thermal correction to Enthalpy=                 0.033007 (Htherm= Etherm+pV)
Thermal correction to Gibbs Free Energy=        0.008252 (Gtherm= Htherm–TS)
Sum of electronic and zero-point Energies= -113.837121(E0=Eelect+ZPE)
Sum of electronic and thermal Energies=    -113.834268 (E= E0+Etrans+Erot+Evib= Eelect +Etherm)
Sum of electronic and thermal Enthalpies=  -113.833324 (H= E+pV= Eelect+Htherm)
Sum of electronic and thermal Free Energies=-113.858079 (G= H–TS= Eelect+Gtherm)
```

The sum of electronic and thermal energies is the same as the internal energy we denoted U above. The expressions on the right also give you options for calculating the thermodynamic quantities, U, H and G.As part of the vibrational analysis, the enthalpies and Gibbs free energies and are evaluatedbased on the molecular mass, molecular geometry and vibrational frequencies. Also, breakdownof thermal energy and entropy among different degrees of freedom are given.

Another example shown here is the isomerisation reaction of hydrogen cyanide to hydrogen isocyanide

HCN ⟶ HNC

(Reactant) (Product)

The relevant partfor the reactant HCN and product HNC are shown below:

For HCN

Sum of electronic and thermal Free Energies= -93.263374 Ha

For HNC

Sum of electronic and thermal Free Energies= -93.23530 Ha

From the Gibbs free energy values, one can calculate the reaction freeenergy using the expression

$$\Delta G_g = \sum G_{products} - \sum G_{reactants} \quad (3)$$

In the following calculation change in Gibbs free energy value of isomerization reaction is converted from Ha unit to kcal/moluint by multiplying Ha value with 627.5095

ΔG = 627.5095*(-93.235305 - (-93.263374)) = 17.6 kcal/mol

Methodology of Current Project

The pKa value of an organic molecule is related to the Gibbs free energy change (ΔGaq) of its deprotonation reaction in aq. medium by the following expression [2,3,4]

$$pKa = \frac{\Delta G_{aq}}{2.303\log(0)} = \frac{\Delta G_q}{1.365} \quad (4)$$

Where Δ Gaq = ΔGg + ΔΔGsolv

(for the deprotonation reaction AH →A-+ H+, where AH the neutral organic molecule and A- is the anion.

ΔGgis the Gibbs free energy of the reaction in gaseous phase calculated using the following scheme

ΔGg=G(A-)+ G(H+)–G(AH) (5)

ΔΔGsolv is the Gibbs free energy of solvation involving the species in the de-protonation reaction. In the current methodology we calculated G(A-)and G(AH) using HF/6-31G computational method. We use the values of G(H+) and ΔΔG solv available in the literature. We calculated the pKa of organic molecules such as Trifluoromethane, Ethylene, Cyclopropane, Phenol, Methane, Ethanol and Benzoic acid in the current work.

Results and Discussion

In this section, we shall present and discuss the results of our calculations in several gaseous phase reactions outlined above. All the results are summarized in the Table I.

Table 1 Free energy values and pka values of organic molecules studied by HF\6-31G are reported here. The energy values are reported in kcal.mol^{-1}. The experimental pKa values are given in brackets along with calculated values. Solvent Phase Values are also reported.

Molecul	ΔG(AH) Ha	ΔGsol (AH) Ha	ΔG(A-) Ha	ΔG(A-) sol Ha	ΔGg kcal/ mol	ΔΔGsolv (Ref 2,3) kcal/ mol	ΔGaq kcal/ mol	pKa
Trifluo-romethane	-338.357	-338.361	-337.761	-337.859	369.73	-324.09	45.633	33.45 (32.0)
Ethylene	-78.591	-78.59	-77.93	-78.04	372.89	-329.74	61.0	44.4 (44.0)
Cyclo-propane	-117.87	-117.88	-117.22	-117.32	407.44	-327.173	80.26	57 (47.0)
Phenol	-307.490	-307.499	-306.94	-307.04	337.28	-321.748	15.53	11.38 (10.0)
Methane	-40.180	-40.182	-39.50	-39.61	419.29	-333.260	86.03	63(48)
Ethanol	-155.05	-155.06	-154.45	-154.57	369.66	-336.244	33.42	24.49 (16.0)
benzoic acid	-420.88	-420.89	-420.34	-420.45	331.88	-327.521	6.25	4.5 (4.2)

We focus on validating the computational chemistry methods in the area of modeling of gaseous phase reactions and calculation of pKa values. The present work can be considered as a benchmark of performingpKa measurements through experimental and computational methods.

Experimental thermochemical data and pKa of molecules are available in standard text books and NIST data base. From the previous computational studies it was observed that HF method over-estimates the electronic energy values. However Smith and coworkers successfully and accurately carried out the calculations of ionization energy, electron affinity and proton affinity of simple gaseous molecules using HF/6-31G method within the range of 3 kJ/mol from the experimental values. The observation motivated us to investigate the gaseous phase reactions involving simple molecules using HF/6-31G method. We finalized the basis set after trial calculations using other split valence basis sets.

In all computational quantum chemistry calculations, electronic structure

calculation is carried out as a function of its coordinates. This is the crucial step in each and every calculation irrespective of the method and nature of the problem. The electronic structures of those molecules are not complicated and thus make the free energy calculation more accurate. When we analyse the calculated pKa values with the experimental values increasing or decreasing trend of pKa values keep consistently. In the case of Trifluoromethane, Ethylene, Phenol and Benzoic acid the difference between calculated and experimental pKa value is only less than 2.0units. However the pKa of cyclopropane, methane and ethanol shows much difference from the experimental value by more than 10 units. This may be attributed to the complex electronic structure and inert nature of methane and cyclopropane.While in the case of ethanol other computational methods may give better approximations to pka calculations. A more accurate calculation of pKa is performedespecially in the case of ethylene and benzoic acid. The difference between the experimental and theoretical results came around an average of 0.3 units.A noticeable result obtained in the case of ethylene where the computational calculation reproduce the experimental result.

A less accurate pKa value is associated with the methane molecule which may be due to the presence of strong C-H bonds which is unavailable for deprotonation. Benzoic acid also give an accurate value with errors less than 1.0 unit. The aromatic nature of benzoic acid and its electronic structure does not affect the accuracy of computational calculation.

Conclusion

In the present work we modeled simple gaseous phase deprotonation reactions and calculated the pKa of organic molecules using HF/6-31G method. The credibility of HF\6-31G method is well documented in the literature. All computational chemistry calculations were performed using Gaussian software. Gaussian software is mainly used in the publication of 75 % research articles in computational chemistry. We obtained accurate results for electron rich species and carboxylic acid in comparison with the experimental data. Thermochemical data obtained from the optimization and frequency analysis of simple gaseous phase systems could be utilized for pKa calculations. However the thermodynamics calculations and reaction modeling using computational quantum chemistry methods are inefficient since thesolvent in the condensed phase reactions are treated implicitly. The incorporation of explicit solvent models and molecular simulations based on classical mechanics is an essential ingredient in pKa calculations.More accurate quantum chemistry methods and codes are also suggested for the extension of the current research work.

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Preliminary study on homestead diversity of medicinal plants in Chundy and Elavoor, Angamaly

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Abstract

This study was carried out for three months on the medicinal plants available around the home hold areas of investigators at Chundy and Elavoor. Medicinal plants belong to 17 families were identified and of which four plants were belonging to family Astraceae.

Introduction

Plants have been used for medicinal purposes long before prehistoric period. Ancient Unani manuscripts, Egyptian papyrus and Chinese writings described the use of herbs. Indigenous cultures such as Rome, Egypt, Iran, Africa and America used herbs in their healing rituals, while other developed traditional medical systems such as Unani, Ayurveda and Chinese Medicine in which herbal therapies were used systematically (Preetha *et*. *al.,* 2015).

Traditional systems of medicine continue to be widely practiced on many accounts. Population rise, inadequate supply of drugs, prohibitive cost of treatments, side effects of several synthetic drugs and development of resistance to currently used drugs for infectious diseases have led to increased emphasis on the use of plant materials as a source of medicines for a wide variety of human ailments.

Among ancient civilizations, India has been known to be rich repository of medicinal plants. The forest in India is the principal repository of large number of medicinal and aromatic plants, which are largely collected as raw materials for manufacture of drugs and perfumery products. About 8,000 herbal remedies have been codified in AYUSH systems in INDIA (Subrat *et*.al, 2002). Ayurveda, Unani, Siddha and Folk (tribal) medicines are the major systems of indigenous medicines. Among these systems, Ayurveda and Unani Medicine are most developed and widely practiced in India.

Recently, WHO (World Health Organization) estimated that 80 percent of people worldwide rely on herbal medicines for some aspect of their primary health care needs. According to WHO, around 21,000 plant species have the potential for being used as medicinal plants (Tewari, 2002).

As per data available over three-quarters of the world population relies mainly on plants and plant extracts for their health care needs. It has been estimated, that in developed countries such as United States, plant drugs constitute as much as 25% of the total drugs, while in fast developing countries such as India and China, the contribution is as much as 80%. Thus, the economic importance of medicinal plants is much more to countries such as India than to rest of the world. These countries provide two third of the plants used in modern system of medi-

cine and the health care system of rural population depend on indigenous systems of medicine (Ved and Goraya, 2009).

Treatment with medicinal plants is considered very safe as there is no or minimal side effects. These remedies are in sync with nature, which is the biggest advantage. The golden fact is that, use of herbal treatments is independent of any age groups and the sexes.

The ancient scholars only believed that herbs are only solutions to cure a number of health related problems and diseases. They conducted thorough study about the same, experimented to arrive at accurate conclusions about the efficacy of different herbs that have medicinal value. Most of the drugs, thus formulated, are free of side effects or reactions. This is the reason why herbal treatment is growing in popularity across the globe. These herbs that have medicinal quality provide rational means for the treatment of many internal diseases, which are otherwise considered difficult to cure.

Apart from the medicinal uses, herbs are also used in natural dye, pest control, food, perfume, tea and so on. In many countries different kinds of medicinal plants/ herbs are used to keep ants, flies, mice and flee away from homes and offices. Now a day's medicinal herbs are important sources for pharmaceutical manufacturing.Recipes for the treatment of common ailments such as diarrhoea, constipation, hypertension, low sperm count, dysentery and weak penile erection, piles, coated tongue, menstrual disorders, bronchial asthma, leucorrhoea and fevers are given by the traditional medicine practitioners very effectively.

Over the past two decades, there has been a tremendous increase in the use of herbal medicine; however, there is still a significant lack of research data in this field. Therefore since 1999, WHO has published three volumes of the WHO monographs on selected medicinal plants.However, development of plants or extracts having potential medicinal uses is blunted by weak scientific evidence, poor practices in the process of drug development, and insufficient financing (Ahn, 2017).

Materials and methods

The study was carried out for three months. The information about medicinal plants around household area of investigators at Chundy, Aluva and Elavoor, Angamaly.Plants were identifiedwith their local name, botanical name, the plant parts used for making medicine and the diseases are cured by them. We made use of experts and books (Thampan, 2015; Meloo,1995) to identify the medicinal plants and to know about their medicinal importance. We conducted field trips to our local home lands to survey the medicinal plants and photographed them for further studies.

Result and discussion

Medicinal plants belong to 17 families were identified during the study period. 4 plants were belonging to family Compositae (Astraceae). The various plant parts are used including leaves, stem, bark, root, flowers and fruits for medicinal use. Leaves were found to be the most commonly used compared to the other parts. For some plants more than one part was found to use medicinally. In general a single plant is used for multiple needs. Various methods of preparations were adopted for its medicinal usage. The medicinal

plants identified in this study and its usage was listed in Table I.

S. No.	PLANT SPECIES & FAMILY	LOCAL NAME
1	Azadirachta indica (Meliaceae)	Aryaveppu
2	Sidacordifolia (Malvaceae)	Kurunthotti
3	Aloe vera (Asphodelaceae)	Kattarvazha
4	Catharanthusroseus (Apocynaceae)	Nithyakalyani/Shavamnari
5	Vernoniacinerea (Compositae)	PoovanKurunthal
6	Wedeliacalendulacea (Astraceae)	Manjakayyonni
7	Massendafrondosa (Rubiaceae)	Vellila
8	Eclipta alba (Asteraceae)	Kayyoni
9	Phyllanthusniruri (Euphorbiaceae)	Keezharnelli
10	Foeniculumvulgare (Apiaceae)	Perunjeeragam
11	Ixora acuminate (Rubiaceae)	AshokaChethi
12	Calendula officinalis (Astraceae)	Bandhi
13	Cyranthusobliquus (Amaryllidaceae)	Umathunga
14	Eucalyptus regnans (Myrtaceae)	Ukkali
15	Ocimum sanctum (Lamiacese)	Thulasi
16	Punicagrantum (Lythraceae)	Mathalanarakam
17	Zingiberofficinale (Zingiberaceae)	Enji
18	Justicaadhatoda (Acanthaceae)	Adalodakam
19	Murrayakoenigii (Rutaceae)	Curryveppila
20	Bacopamonnieri (Plantaginaceae)	Brahmi
21	Alcearosea (Malvaceae)	Majic Rose
22	Crinum bulbispermum (Amaryllidaceae)	Lilly
23	Eugenia caryophyllata (Myrtaceae)	Gramboo
24	Optuniaaurantiaca (Cactaceae)	Kallimulchedi
25	Menthapiperita (Lamiaceae)	Puthina

Discussion

Medicinal Plants constitute an important component of the plant resource spectrum of Kerala. Recent analysis shows that out of estimated 4600 flowering plants in Kerala, about 900 possess medicinal values. Of these, 540 species are reported to occur in forest ecosystems. Over 150 species of plants that are either indigenous or naturalized in Kerala are used in the Indian system of Medicine like Ayurveda and Sidha. The rural folk and tribal communities make use of about 2,000 species of lesser-known wild plants for various medicinal uses. About 60 to 65% of plants required for Ayurvedic medicine and almost 80% of plants used in Sidha medicine are found in the forests of

Kerala (www.keralaforest.org).

Medicinal plants, also called medicinal herbs, have been discovered and used in traditional medicine practices since prehistoric times. Plantssynthesize hundreds of chemical compounds for functions including defense against insects, fungi, diseases, and herbivorous mammals. Numerous phytochemicals with potential or established biological activityhave been identified. The phytochemical content and pharmacological actions of many plants having medicinal potential remain unassisted by scientific research to define efficacy and safety (Ahn, 2017).

Medicinal plants are widely used in non-industrialized societies, mainly because they are readily available and cheaper than modern medicines. The annual global export value of 50,000 to 70,000 types of plants with suspected medicinal properties was estimated to be US$2.2 billion in 2012(Medicinal and aromatic Programme, 2017) and in 2017, the potential global market for botanical extracts and medicines was estimated at several hundred billion dollars (Ahn, 2017). In many countries, there is little regulation of traditional medicine, but the World Health Organization coordinates a network to encourage safe and rational usage. Medicinal plants face both general threats, such as climate change and habitat destruction, and the specific threat of over-collection to meet market demand (Ahn, 2017).

Drug research makes use of ethnobotany to search for pharmacologically active substances in nature, and has in this way discovered hundreds of useful compounds. These include the common drugs aspirin, digoxin, quinine, and opium. The compounds found in plants are of many kinds, but most are in four major biochemical classes: alkaloids, glycosides, polyphenols, and terpenes.

Conclusion

As our lifestyle is now getting techno-savvy, we are moving away from nature. As herbs are natural products they are free from side effects, they are comparatively safe, eco-friendly and locally available. Traditionally there is lot of herbs used for the ailments related to different seasons. There is a need to promote them to save the human lives.In many of the developing countries the use of plant drugs is increasing because modern life saving drugs are beyond the reach of three quarters of the third world's population although many such countries spend 40-50% of their total wealth 4 on drugs and health care. As a part of the strategy to reduce the financial burden on developing countries, it is obvious that an increased use of plant drugs will be followed in the future.

These herbal products are today are the symbol of safety in contrast to the synthetic drugs, that are regarded as unsafe to human being and environment. Although herbs had been priced for their medicinal, flavouring and aromatic qualities for centuries, the synthetic products of the modern age surpassed their importance, for a while. However, the blind dependence on synthetics is over and people are returning to the naturals with hope of safety and security. It's time to promote them globally.

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