

“EXTRACTION OF CAFFEINE FROM SOME TEA AND COFFEE SAMPLES”

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Abstract : Caffeine is an alkaloid and a member of the xanthine family. It is odourless, non-toxic, has a bitter taste and is highly soluble in hot water. Caffeine occurs naturally in coffee, tea, cocoa, mate, kola nuts and a variety of other plants. Some plant species that contain caffeine such as tea and coffee may also contain trace amounts of another alkaloid called theophylline. Caffeine is bioactive and in moderation, it has beneficial effects on the body; it increases alertness, serves as a bronchial dilator, stimulates metabolism and contributes to an increase in dopamine levels in the blood, which improves mood. Whereas caffeine is a natural constituent in coffee, tea, chocolate, and some cola drinks, it is added to consumer products such as soft drinks, diet pills, and analgesics. Caffeine is said to be the most widely used drug in the world. It has pharmacological uses as a cardiac and respiratory stimulant and as an agent that promotes kidney diuresis. There may be some adverse effects due to excessive caffeine intake, such as restlessness, headaches, heart palpitations, heartburn, and insomnia.

Index terms : Caffeine, Xanthoid, Extraction.

INTRODUCTION

Caffeine is an alkaloid. Generally, caffeine is found in coffee and tea based beverages and products, chocolate based beverages and products, sodas, energy drinks, energy shots, and a wide range of supplements including pain relievers as well as workout supplements.

Tea is the most commonly and widely used soft beverage in the household. It originated in the south-western China, where it was used as a medicinal drink. It was popularized as a recreational drink during the Chinese Tang dynasty and tea drinking spread to other East Asian countries. Portuguese priests and merchants introduced it to the west during the sixteenth century. During the 17th century, drinking tea became fashionable among Britons, who started large scale production and commercialization of the plant in India.

Tea belongs to the family *Camelliaceae* and all the cultivated tea plants belong to two distinct species, viz. *Camelliasinensis*, the short leaved China plants and *Camellia assamica*, the broad leaved Assam plants. Tea prefers a warm humid climate, well distributed rainfall and long sunshine days. A soil pH below 6 is essential for establishing tea successfully and moderately good tea can be grown on soils with pH values between 4.5 and 5.5. Under natural conditions this plant grows to a small tree, but brought into a bush form by

pruning at regular intervals for the convenience for plucking and harvesting optimum growth. Australia, Argentina, Bangladesh, China and India are some of the tea growing countries. In south India, Wayanadu, The Nilgiris(Tamil Nadu), Coorg (Karnataka), Haasan (Karnataka), Nelliampathy(Kerala) and Anamallais are the most important tea growing places.

Coffee is another widely used beverage. It is a brewed drink prepared from roasted coffee beans, which are the seeds of berries from the coffee plant [1-3]. The plant is native to subtropical Africa and some islands in southern Asia. The two most commonly grown are the highly regarded *Coffea arabica* and the less sophisticated, but stronger and hardier *robusta*(*Coffeacanehora*) and they are classified in Rubiaceae family. Once ripe, coffee beans are picked, processed and dried. Dried coffee beans are roasted to varying degrees, depending on the desired flavor. Roasted beans are grounded and brewed to produce coffee as a beverage. Coffee seeds contain caffeine from 1-2%, together with tannin, glucose, fats and proteins.

Such beverages are mainly used in order to remove fatigue, tiredness and headache. It acts as a stimulant for CNS(Central Nervous System) and skeletal muscles. It also increases the capacity of thinking. It is also used for lowering body temperature [4-8]. All these properties are attributed to the chemical composition of these beverages (tea leaves and coffee seeds).

Tea shoot contains a full complement of enzymes, biochemical intermediates, carbohydrates, proteins and lipids. In addition, tea shoot is distinguished by its remarkable content of polyphenols and methyl xanthenes (caffeine and other purines such as theobromine and theophylline). Popularity of tea and coffee as beverages may be due to the presence of these two groups of compounds which are mainly responsible for their unique taste, in addition to various compounds associated with their aroma. Chemical composition of tea shoot varies with agroclimatic condition, season, cultural practice and the type of material.

Flavanols, flavanol glycosides, polyphenolic acids and depsides put together are referred to as total polyphenols and make up about 80% of the dry weight in a tea shoot. Flavanols or catechins are the major compounds that are oxidizable in the tea leaf.

Quality of tea is determined by the presence or absence of chemical compounds which impart colour, briskness, brightness, strength and flavor in the infusion. Majority of the chemicals imparting quality are produced during the processing of tea leaves. Biogenesis of such precursors is influenced on one hand by the genetic and environmental factors which can't be controlled and on the other hand by the cultural practices adopted in the field as well as by the conditions of processing, which can be controlled. Though biochemical changes start immediately after plucking(the crop shoots) the precise changes required for the quality starts from withering onwards.

Theaflavins are orange red substances that contribute significantly to the astringency, briskness, brightness and colour of the tea beverage. TF of black tea comprise a number of

fractions namely theaflavin, theaflavin monogallate and digallate, epitheaflavic acid and isotheaflavin. Thearubigins are complete condensation products of oxidized catechins with theaflavins. Together with HPS,TR contributes to the colour,mouth feel and body of the tea liquor. Caffeine is relatively a stable molecule and is a direct stimulant of the CNS. Together with Tf, it imparts briskness to the liquor.High levels of caffeine indicate a good leaf standard. Caffeine decreases with the maturity of the crop shoots. Volatile flavour constituents, in addition to the biochemical constituents give the tea its unique taste.

WHAT IS 'CAFFEINE'?

Caffeine, originally called 'thein' was first discovered in tea in 1827. It was later shown that the 'thein' of tea was identical with the caffeine of coffee and the term 'theine' was then dropped. It belongs to the family of heterocyclic compounds known as purines. It can be classified as an alkaloid. It is a xanthine alkaloid. Many of the stimulants are derived from xanthine. Caffeine is named systematically as 1,3,7-trimethylxanthine or 3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione. Caffeine occurs as a white powder or as needles and has bitter taste.

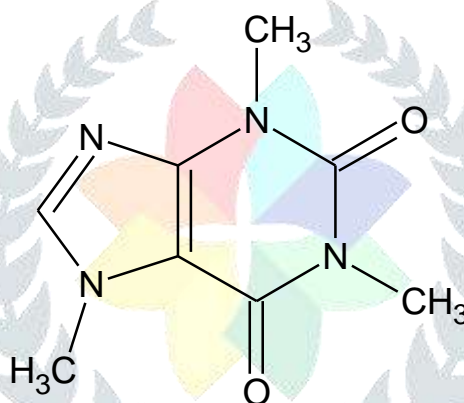


Fig.1.1. Structure of caffeine

Pharmacology

Pharmacodynamics:

A little adenosine is present in the neurons of Central Nervous System (CNS) even though caffeine is absent in our body and we remain awake and alert. If this awake and alert condition persists for a long time, it results in the accumulation of adenosine in the neuronal synapse increases and it will activate the adenosine receptors present on certain CNS neurons, when the adenosine receptors are activated, it will produce a cellular response which increases drowsiness. But when caffeine is consumed, it will suppress the activation of adenosine receptors by blocking the location on the receptor where adenosine binds to it. As a result, caffeine provides a temporary relief from drowsiness and makes the person energetic to some extent [9-11].

Structure of A Typical Chemical Synapse:

Caffeine is a receptor antagonist to all adenosine receptors. This antagonism will stimulate the medullary vagal, respiratory centers etc which increase the respiration rate reduces heart rates etc. Adenosine acts as an inhibitory neurotransmitter that suppresses activity in the central nervous system. Since caffeine is both water and lipid soluble, it readily diffuses through the blood – brain barrier that separates the blood stream from the interior of the brain. Once it enters the brain, it will act as an antagonist for the adenosine receptors present in the brain. The caffeine molecule is structurally similar to adenosine, so it is capable of binding to adenosine receptors present on the surface of the cell without activating them.

Even though caffeine does not bind directly to any dopamine receptors, it influence the binding activity of dopamine at its receptors in the striatum by binding to adenosine receptors that have formed GPCR heteromers with dopamine receptors. Caffeine, like other xanthenes, acts as a phosphodiesterase inhibitor and thereby raises intracellular cAMP, activates proteins Kinase A, inhibits TNF – alpha and leukotriene synthesis and reduces inflammation and innate immunity.

Pharmacokinetics:

Caffeine that reaches our body through coffee and other beverages is absorbed by the small intestine within 45 minutes of ingestion and distributed to all body tissues. Peak blood concentration is reached within 1-2 hours and it is eliminated by first order kinetics. The biological half life of caffeine, i.e. the time required for the body to eliminate one half of the dose varies among individuals – depending upon the factors like pregnancy, use of other drugs, liver enzyme function level and age. In healthy adults, half life of caffeine is between 3-7 hours. Nicotine decreases the half life by 30-50% while oral contraceptives and double it. Pregnancy can raise the half life of caffeine as much as 15 hours during the last trimester. In newborns, the half life can be 80 hours or more.

Caffeine is metabolized in the liver into three primary metabolites;

- **Paraxanthine (84%)**: Increase lipolysis, leading to the increased level of glycerol and free fatty acid levels in blood plasma.
- **Theobromine (12%)**: Dilate the blood vessels and increases urine volume.
- **Theophylline (4%)**: Relaxes smooth muscles of the bronchi and is used for the asthma treatment.

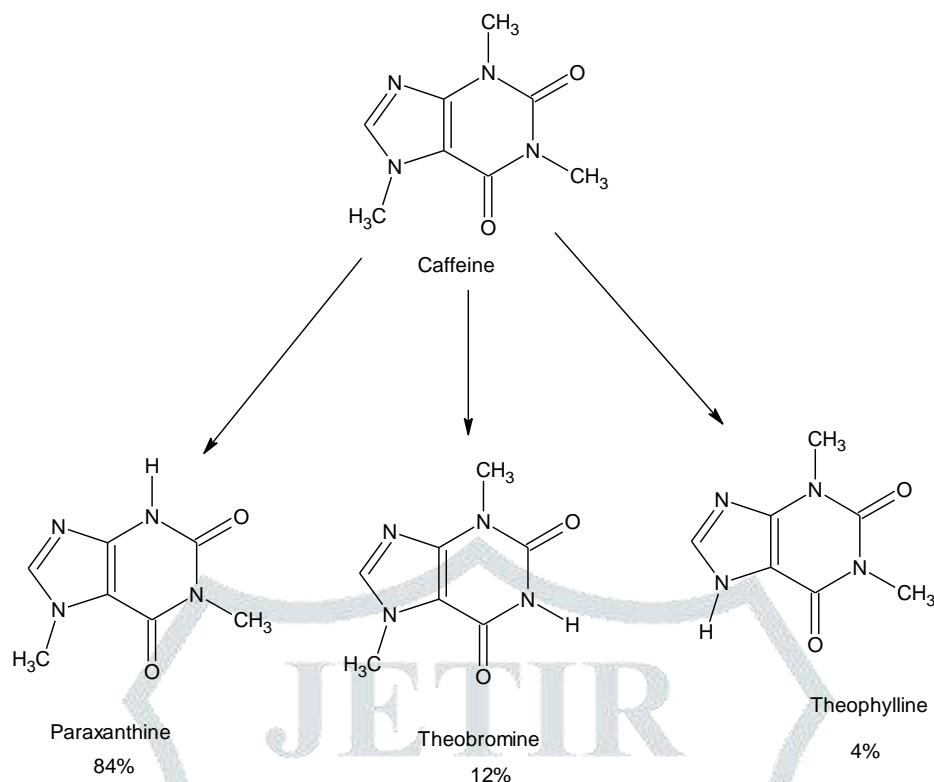


Fig.1.2. Metabolism of caffeine

USES

1. Medical

- a. Brochopulmonary dysplasia in premature infants can be prevented or can be treated. It may improve weight gain during therapy and reduce the incidence of cerebral palsy.
- b. To treat apnea of prematurity.
- c. Orthostatic hypotension treatment.

2. Enhancing Performance:

Caffeine is a CNS and metabolic stimulant and it will reduce the awake and drowsiness feel to the people. The consumption of caffeine will increase our focus and general body coordination. But the amount of caffeine needed to produce these effects will be different from person to person depending upon their physical status.

3. Neurological conditions

Caffeine is believed to help prevent or delay Alzheimer's disease, and Parkinson's Disease as well as treat some types of hyperactivity disorders.

4. Pain relief

Caffeine reduces inflammation and helps to block the perception of pain in the brain. Coffee drinks are among the most popular sources of caffeine, believed to be the most commonly used drug worldwide.

Epinephrine and glucagon—hormones that initiate the "fight or flight" response in animals are also highly stimulated by caffeine. Other proposed mechanisms have to do with effects on CNS intracellular calcium ion concentrations.

Caffeine also creates an effect of preventing sleep, but do not affect the people in the same way. In athletes, moderate doses of caffeine improve sprint, stamina and team sports performance. But coffee does not produce as much as enhancing effects observed in other sources. The consumption of caffeine has both beneficial and harmful effects depending on the nature of the task [12-13].

Effect on Specific Populations

- Adolescents and Adults

The amount of caffeine intake for this age group should be not more than 2.5mg /kg body weight. This is because the maximum caffeine does will not be appropriate for younger adults who are still growing. So the daily dose of 2.5mg/kg body weight would not cause any adverse health effects in the majority of adolescent caffeine consumers.

- Children

Caffeine intake by healthy children produces modest and typically innocuous effects. For children age 12 and under the caffeine intake should not be more than 2.5mg /kg body weight. But based on the average body weights of the children, the intake limits are listed below.

Table 1.1

Age Range	Maximum recommended caffeine in take
4-6	45 mg
7-9	62.5mg
10-12	85mg

Recently, studies shows that caffeine can be used to treat hyperkinetic children. Researchers found that 200-300mg of caffeine has a similar effect to methylphenidate for the treatment of hyperkinetic impulse disorder. Also, caffeine treatment does not show any side effects caused by methylphenidate.

Over Dose

Consumption of 1-1.5g per day causes a condition called caffeineism. It is accompanied with a series of unpleasant symptoms including nervousness, restlessness, headaches and palpitations. Over dose of caffeine can also causes a state of over – stimulation of central nervous system called caffeine intoxication. This syndrome occurs only during the ingestion of caffeinated beverages and tablets which contain over amount of caffeine. The symptoms of caffeine intoxication includes restlessness, fidgeting, anxiety, excitement increased urination, gastrointestinal disturbance muscle twitching, irritability and irregular, rapid heartbeat. Massive over dose can cause death. Treatment of severe caffeine intoxication includes peritoneal dialysis, hemodialysis and hemo filtration.

Side Effects

- **Physical**

Caffeine will increase blood pressure and cause vasoconstriction. Long term consumption of caffeine is associated with chronic arterial stiffness. It will also affect gastrointestinal motility and gastric acid secretion. Caffeine increases basal metabolic rates in adults. In postmenopausal women, high caffeine consumption can accelerate bone loss. The increased use of caffeine also increases the urinary output which increases the risk of dehydration. Caffeine in low doses may cause weak bronchodilation for up to four hours in asthmatics. Also, studies have shown no correlation between caffeine intake and increased risk of osteoporosis or increased risk of spontaneous abortion. Caffeine enters the bloodstream about ten minutes after its ingestion and stays in the body for up to twelve hours [14-15].

- **Psychological**

Psychological symptoms arise due to caffeine consumption includes anxiety and reduced co-ordination. At higher doses, typically greater than 300mg, caffeine can cause anxiety and panic disorders. But low doses of caffeine can increase alertness and decreased fatigue.

- **During Pregnancy**

The consumption of caffeine during pregnancy does not increase the risk of miscarriage or growth retardation even consumed in moderate to high amounts the UK food standard agency recommended that pregnant women should limit their caffeine intake to less than 200mg a day. Even though our consumption of caffeine is harmful during pregnancy, there is some evidence that the hormonal changes during pregnancy slow the metabolic clearance of caffeine from the system, causing a given dose to have long lasting effects.

- **Reinforcement disorders**

Certain users can become addicted and therefore unable to decrease the use of caffeine even though they know the negative effects of the queues of caffeine.

- **Jitters**

In some people, caffeine causes moderate to severe shaking of the hands. Mild physical dependence arises due to repeated daily intake of caffeine. It causes fatigue, headache, sleepness or drowsiness (Insomnia), stomach pain and joint pain. Withdrawal headaches are experienced by roughly half of those who stop consuming caffeine for two days following an average intake of 235g. Tolerance to some undesired effects, particularly to caffeine's autonomic effects, develops quickly among heavy coffee and energy drink consumers.

Gene polymorphism can be associated with withdrawal symptoms and beta-1 and beta-2 play a major role in caffeine withdrawal. For example, compared to people with homozygous gly16 allele, consumers with the heterocygote ADR beta-2 Gly 16 Arg gene polymorphism having a higher chance of feeling fatigue after 48 hours of caffeine withdrawal. It is found that beta-2 adrenoceptors are the main cause for this increase in mental fatigue symptoms. Beta -2 adrenoceptors are receptors that regulate glycogenolysis, secrete insulin and intramuscularly transport glucose that is used for cerebral and muscle activity.

Coffee consumption is associated with a lower overall risk of cancer and heavy coffee consumption may increase the risk of bladder cancer. A protective effect of caffeine against Alzheimer's disease is also possible. It will also increase the risk of cardiovascular diseases. Caffeine increases intraocular pressure in those with glaucoma. Caffeine may increase the effectiveness of some medications including one used to treat headaches. Originally caffeine was only ingested through the consumption of plant parts that naturally contain caffeine, but food scientists began synthesizing caffeine as an additive for all kinds of beverages and foods [16].

The Addictive Nature of Caffeine

One of the most prominent issues surrounding the use of caffeine is its addictive nature. Caffeine addiction can range from mild to severe and most of the time it is an addiction most people can live a healthy life with. This is not the case when dangerous amounts of caffeine are being consumed daily or if caffeine is consumed through sugary beverages, which are linked to obesity and type 2 diabetes. Cutting back on caffeine would be recommended for anyone who begins to consume amounts exceeding what is recommended as safe or if getting enough caffeine interferes with work or daily functioning.

The Industry

Despite the problems associated with caffeine use, don't expect humans to quit using it any time soon. According to the International Coffee Organization coffee alone is a 60 billion dollar industry world-wide and the energy drink/energy shot industry is worth over 13 billion in the USA alone. There is huge money in keeping people caffeinated and consumer demand has never been greater since China is now turning on to espresso based coffee. All of this money means that the industry has huge influence on lawmakers and food policy, so any new regulations involving caffeinated products will likely be small. However, expect stricter caffeine labeling regulations to be issued soon most likely including caffeine amounts and safety warnings.

Education is Paramount

Educating consumers about caffeine is the single most important factor in helping people safely use caffeine. If consumers gain knowledge about the amount of caffeine in the products they consume as well as the dangers associated with consuming too much, then consumers will be able to make educated and responsible decisions regarding caffeine consumption for themselves and any minors under their care. Schools also should build caffeine safety education into their health curriculum, so that caffeine awareness and safety can be ingrained into our culture from an early age.

Caffeine use isn't going stop anytime soon, so understanding how to use caffeine both safely and responsibly is crucial.

Products:

- **Coffee**

The primary source of caffeine is 'coffee bean' from which the coffee is brewed. But the caffeine content in coffee varies depending upon the type of coffee bean and the method of preparation used. For an Arabica variety 'Espresso', one serving of coffee ranges from 80-100 milligrams of caffeine, and for drip coffee, the caffeine content is approximately about 100-125 milligram. In general, dark roast coffee has slightly lesser amount of caffeine than lighter roasts because the roasting process reduces the caffeine content of the bean by a small amount.

- **Tea**

Tea contains more caffeine than coffee by dry weight. Tea contains small amount of the bromine and slightly higher levels of the phylline than coffee. Preparation and many other factors have great impact on tea and colour is a very poor indicator of caffeine content, ie, tea like the pale Japanese green tea, 'gyokuro' contain far more caffeine than much darker teas like 'lapsangsouchong', which has very little.

- **Soft Drinks**

Caffeine is a common ingredient in soft drinks such as cola, originally prepared from kola nuts. Soft drinks contain 0 to 55 mg caffeine per 12 ounce serving. The caffeine in the soft drinks is either produced by the ingredients used or it is an additive derived by chemical synthesis. Guarana, a primary ingredient of energy drinks, contain large amount of caffeine with small amount of theobromine and theophylline in a naturally occurring slow – release experiment.

- **Chocolate**

Chocolate, derived from cocoa contain a small amount of caffeine. The weak stimulant effect of chocolate is due to the combination of theobromine and theophylline, as well as caffeine. For example, 28gm serving of a milk chocolate bar has about as much caffeine as a cup of decaffeinated coffee. By weight, dark chocolate has one to two times the amount caffeine, ie , 80-160 mg per 100 gm.

- **Tablets**

Tablets have many advantages over coffee and tea for convenience. These tablets are commonly used by students studying for their exams and by people who work or drive for long hours.

Some beverages combine alcohol with caffeine. So the stimulant effect of caffeine will mask the depressant effects of alcohol and potentially reducing the awareness of intoxication. Yaba contains a combination of methamphetamine and caffeine.

Society and Culture

The Food and Drug Administration(FDA) allows only beverages containing less than 0.02% caffeine, but caffeine powder, which is sold as a dietary supplement is unregulated. There are number of food ingredients that naturally contain caffeine. Coffee and chocolate are broadly recognized as caffeine sources, some ingredients are likely less recognized as caffeine sources. For these natural sources of caffeine, there is no regulatory provision requiring that a food label identify the presence of neither caffeine nor state the amount of caffeine present in the food.

Global consumption of caffeine has been estimated at 120,000 tons per year, making it the world's most popular psychoactive substance. Some Christian scientists and church adherents do not consume caffeine. They believe that they are not supposed to consume a non-medical, psychoactive substance. Gaudiya Vaishnavas also banned the use of caffeine, because they believe that it clouds the mind and over stimulate the senses. To be initiated under a guru, one must have had no caffeine, alcohol, nicotine or any other drugs for at least a year.

Caffeine is toxic to birds, dogs and cats and also has a pronounced effect on various insects and spiders. This is due to their poor ability to metabolize the compound. Caffeine has been found to enhance the reward memory of honeybees and improving the reproductive success of the pollen producing plants.

OBJECTIVES OF PRESENT WORK

The objectives of present study are,

- a. to isolate caffeine from some commercially available tea and coffee samples
- b. to isolate caffeine content from roasted coffee bean
- c. to compare the amount of caffeine content in the analyzed samples.

Results of this study could be used to obtain satisfactory data on caffeine content in plant materials.

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MATERIALS AND METHODS

The data for the present work comprises three tea and two coffee samples. The tea samples and one coffee sample are drawn from different brands of tea available in India and other coffee sample is derived by grinding coffee seeds.

Materials used:

Available samples of tea powder (Three roses, Red label and AVT), Available samples of coffee powder (Bru and locally available roasted coffee seeds, Distilled water, lead acetate solution (saturated), chloroform etc.

Method:

20g of tea powder was weighed and taken as sample. It was then refluxed with 90ml of distilled water. The residue was again refluxed and filtered. The filtrates obtained were combined. 12.5ml of lead acetate solution was added leading to the formation of a curdy brown coloured precipitate. Again the solution was filtered and 40 ml of chloroform was added in four instalments. After adding chloroform, two layers appeared in the separating funnel. The lower layer was separated and the solution then exposed to atmosphere in order to allow chloroform to get evaporated and the residue left behind was caffeine. It was weighed and melting point was noted. The infrared and UV-Vis spectra of all caffeine samples extracted were recorded. Similar procedure was performed with the other samples too [1-6].

METHODS OF CHARACTERIZATION

Infrared spectroscopy (IR spectroscopy) is the spectroscopy that deals with the infrared region of the electromagnetic spectrum, that is light with a longer wavelength and lower frequency than visible light. It covers a range of techniques, mostly based on absorption spectroscopy. As with all spectroscopic techniques, it can be used to identify and study chemicals. A common laboratory instrument that uses this technique is a Fourier transform infrared (FTIR) spectrometer.

The infrared portion of the electromagnetic spectrum is usually divided into three regions; the near-, mid- and far- infrared, named for their relation to the visible spectrum. The higher-energy near-IR, approximately $14000\text{--}4000\text{ cm}^{-1}$ ($0.8\text{--}2.5\text{ }\mu\text{m}$ wavelength) can excite overtone or harmonic vibrations. The mid-infrared, approximately $4000\text{--}400\text{ cm}^{-1}$ ($2.5\text{--}25\text{ }\mu\text{m}$) may be used to study the fundamental vibrations and associated rotational-

vibrational structure. The far-infrared, approximately $400\text{--}10\text{ cm}^{-1}$ ($25\text{--}1000\text{ }\mu\text{m}$), lying adjacent to the microwave region, has low energy and may be used for rotational spectroscopy. The FTIR instrument used for the characterization studies of the present work was Shimadzu IR Prestige 21.

A little of the caffeine extracted from all the analysed samples were mixed with equal quantity of potassium bromide and absorption in infrared region were measured.

UV-Vis Spectroscopy refers to absorption spectroscopy or reflectance spectroscopy in the ultraviolet-visible spectral region. This means it uses light in the visible and adjacent (near-UV and near-infrared [NIR]) ranges. The absorption or reflectance in the visible range directly affects the perceived color of the chemicals involved. In this region of the electromagnetic spectrum, molecules undergo electronic transitions. UV/Vis spectroscopy is routinely used in analytical chemistry for the quantitative determination of different analytes, such as transition metal ions, highly conjugated organic compounds, and biological macromolecules. Spectroscopic analysis is commonly carried out in solutions but solids and gases may also be studied. The instrument used for the solution state UV Vis spectral characterization studies of the present work was Shimadzu UV 2450 UV Vis spectrophotometer.

A little of extracted caffeine was dissolved in 10 ml of chloroform and taken in a quartz cuvet. UV spectrum was run for this solution and a maximum absorption of in UV and visible region was recorded.

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RESULTS AND DISCUSSION

The caffeine from tea and coffee samples were extracted by early described procedure weighed and melting point was noted. The infrared and UV-Vis spectra of all caffeine samples extracted were recorded.

Sample 1 : caffeine extracted from Three Roses

i. IR spectrum

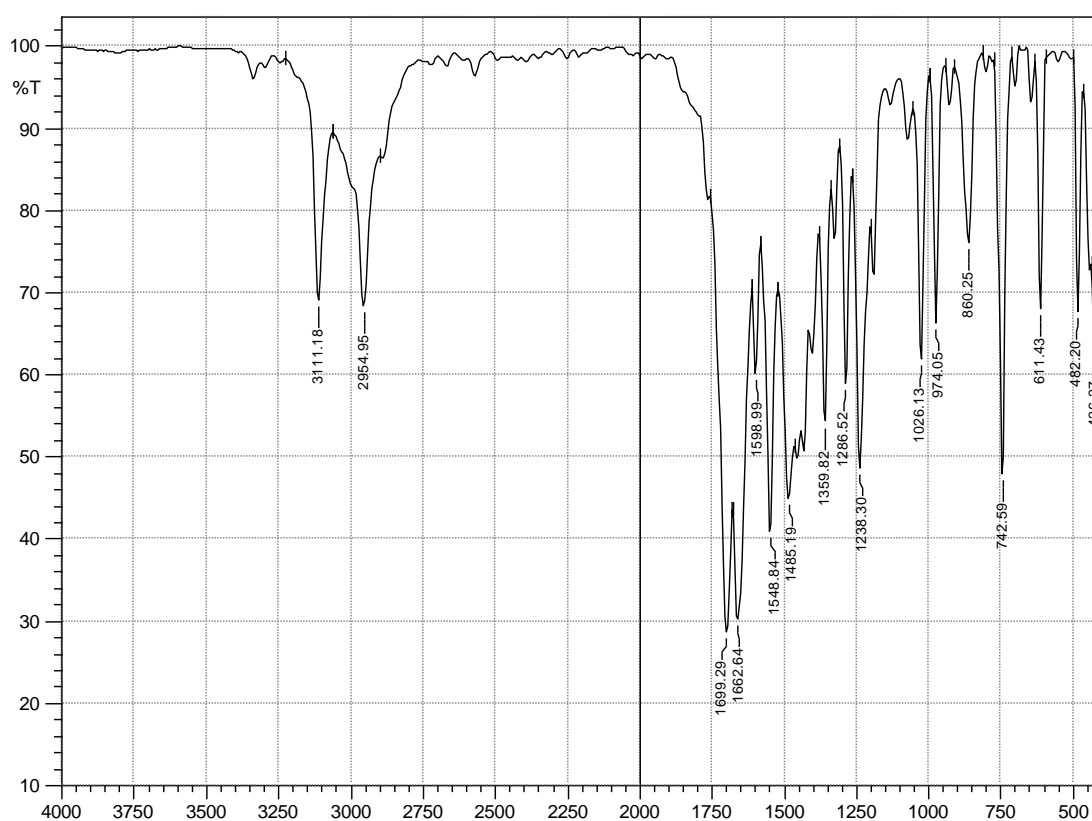


Fig. 3.1

The peaks at 2900-3000 cm^{-1} is assigned to C-H stretching absorptions. Strong peaks found at 1699 and 1662 cm^{-1} are due to C=O and C=N stretching absorptions respectively. The C=C bond skeletal vibrations gave IR absorption at $\bar{\nu}$ 1548 cm^{-1} and the strong peak at $\bar{\nu}$ 1238 cm^{-1} is assigned to C-N stretching absorption. All these observations are in good agreement with the IR spectral data of standard caffeine sample [1].

ii. UV – Vis Spectrum

Purines give sharp absorption at 270nm, but in caffeine the absorption is shifted into 275nm, due to substitution of three methyl groups on three nitrogen atoms. The appearance of absorption band at 275nm for caffeine is attributed to the electronic transition of $n \rightarrow \sigma^*$ and $\pi \rightarrow \pi^*$ where unpaired electrons are available in excess on nitrogen atoms and carbonyl groups in addition to double bonds. The absorption band seen at 237 nm is assigned to the $\pi \rightarrow \pi^*$ electronic transitions of C=C. The observations are in close agreement with the absorption bands in the standard samples of caffeine [2].

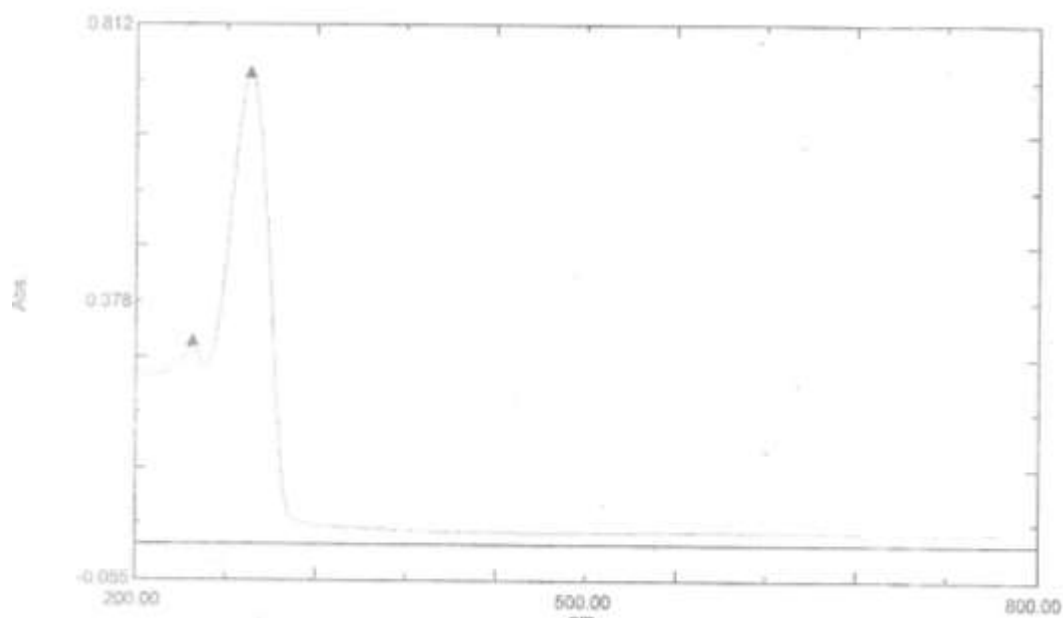


Fig. 3.2

Sample 2: caffeine extracted from AVT

i. IR spectrum

IR spectrum of the sample extracted from the brand AVT premium tea also agrees with the data of standard caffeine sample. The peaks at $2900-3000 \text{ cm}^{-1}$ is assigned to C-H stretching absorptions. Strong peaks found at 1699 and 1660 cm^{-1} are due to C=O and C=N stretching absorptions respectively. The C=C bond skeletal vibrations gave IR absorption at $\bar{\nu} 1548 \text{ cm}^{-1}$ and the strong peak at $\bar{\nu} 1238 \text{ cm}^{-1}$ is assigned to C-N stretching absorption.

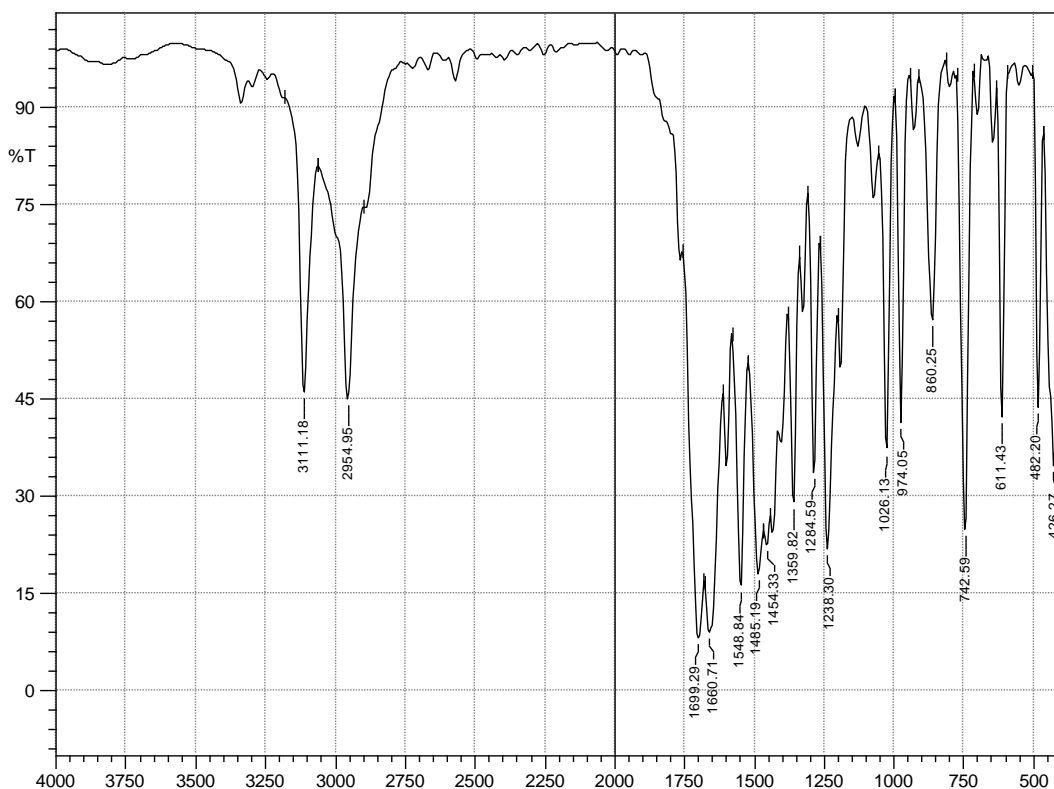


Fig. 3.3

ii. UV Vis Spectrum

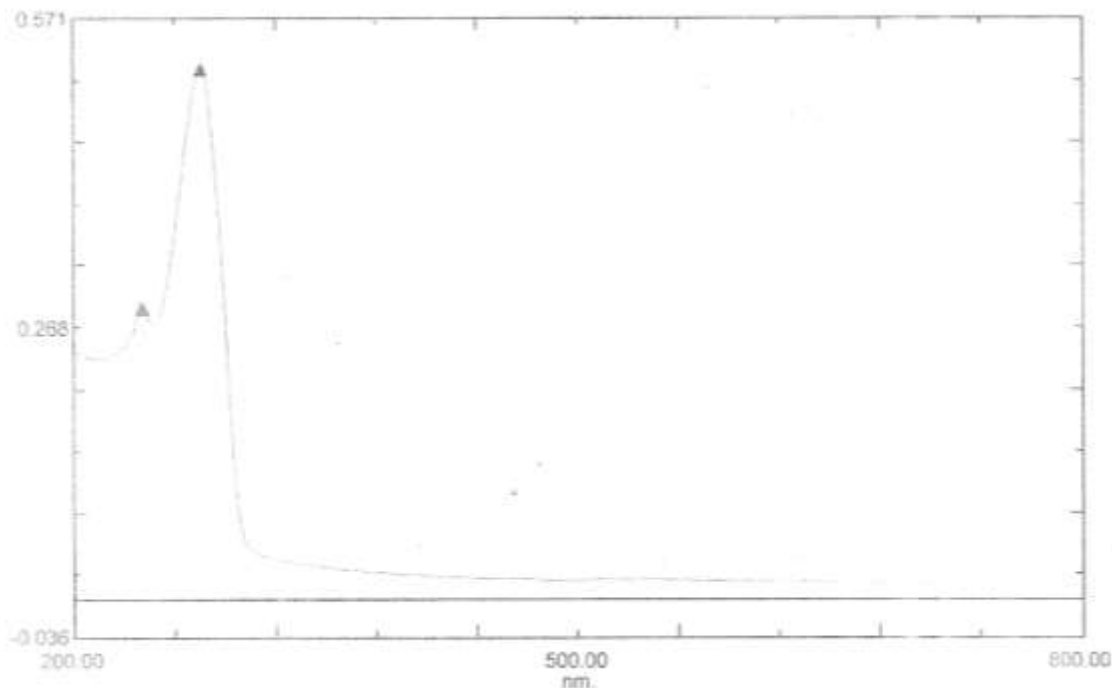


Fig. 3.4

Here in the absorption bands are at λ values 275 nm and 241 nm due to the electronic absorptions of N-H, C=O and C=C functional groups, in agreement with the standard sample of caffeine.

Sample 3: caffeine extracted from Ripple tea

i. IR spectrum

The peaks at 2900-3000 cm^{-1} is assigned to C-H stretching absorptions. Strong peaks found at 1701 and 1660 cm^{-1} are due to C=O and C=N stretching absorptions respectively. The C=C bond skeletal vibrations gave IR absorption at $\bar{\nu}$ 1548 cm^{-1} and the strong peak at $\bar{\nu}$ 1238 cm^{-1} is assigned to C-N stretching absorption. Here also the spectrum confirms caffeine structure as it is in close agreement with the standard sample.

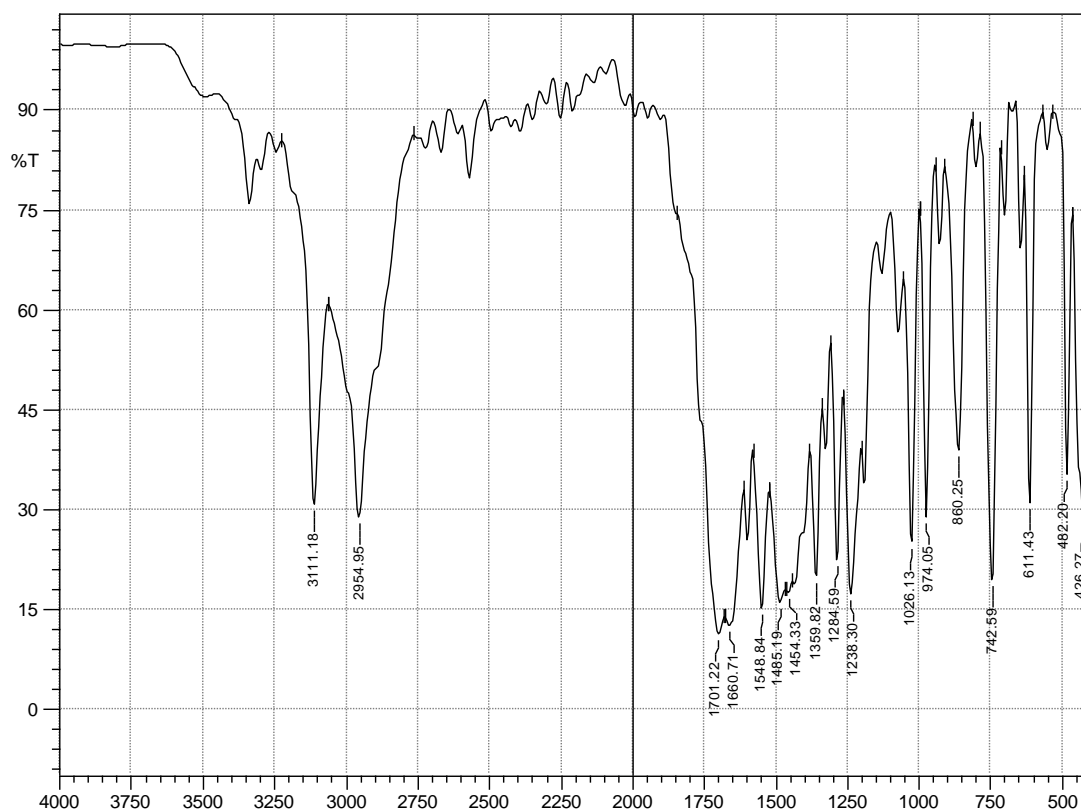


Fig. 3.5

ii. UV Vis Spectrum

UV-Vis spectrum of caffeine sample extracted from Ripple tea gave electronic absorption bands at λ values 275 nm and 239 nm, similar to those extracted from the samples discussed earlier.

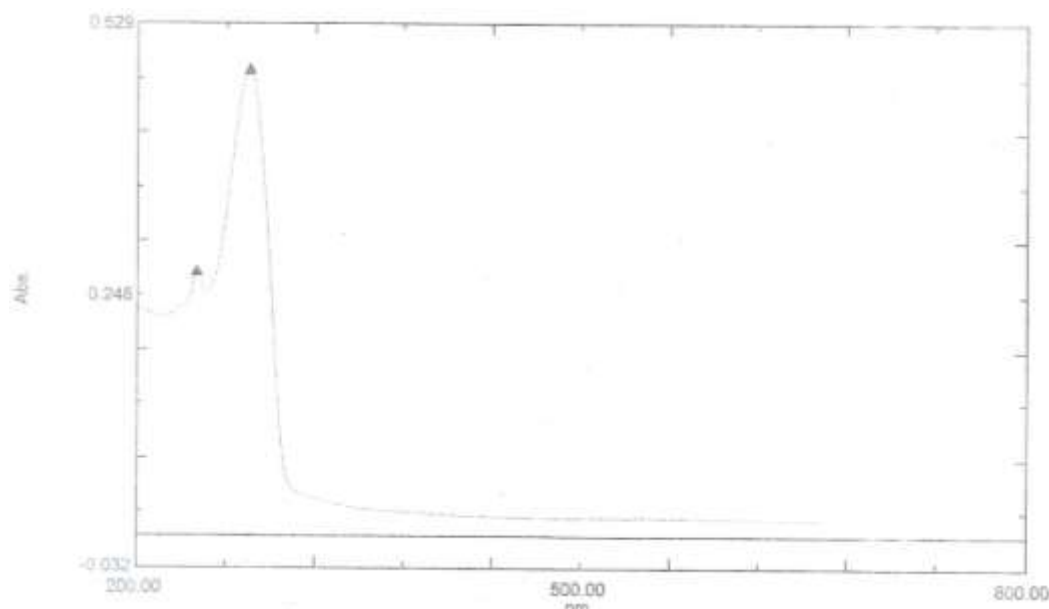


Fig. 3.6

Sample 4: caffeine extracted from Bru coffee

i. IR spectrum

The peaks at 2951 and 3113 cm^{-1} is assigned to C-H stretching absorptions. Strong peaks found at 1699 and 1660 cm^{-1} are due to C=O and C=N stretching absorptions respectively. The C=C bond skeletal vibrations gave IR absorption at $\bar{\nu}$ 1550 cm^{-1} and the strong peak at $\bar{\nu}$ 1238 cm^{-1} is assigned to C-N stretching absorption. Here also the spectrum confirms caffeine structure as it is in close agreement with the standard sample.

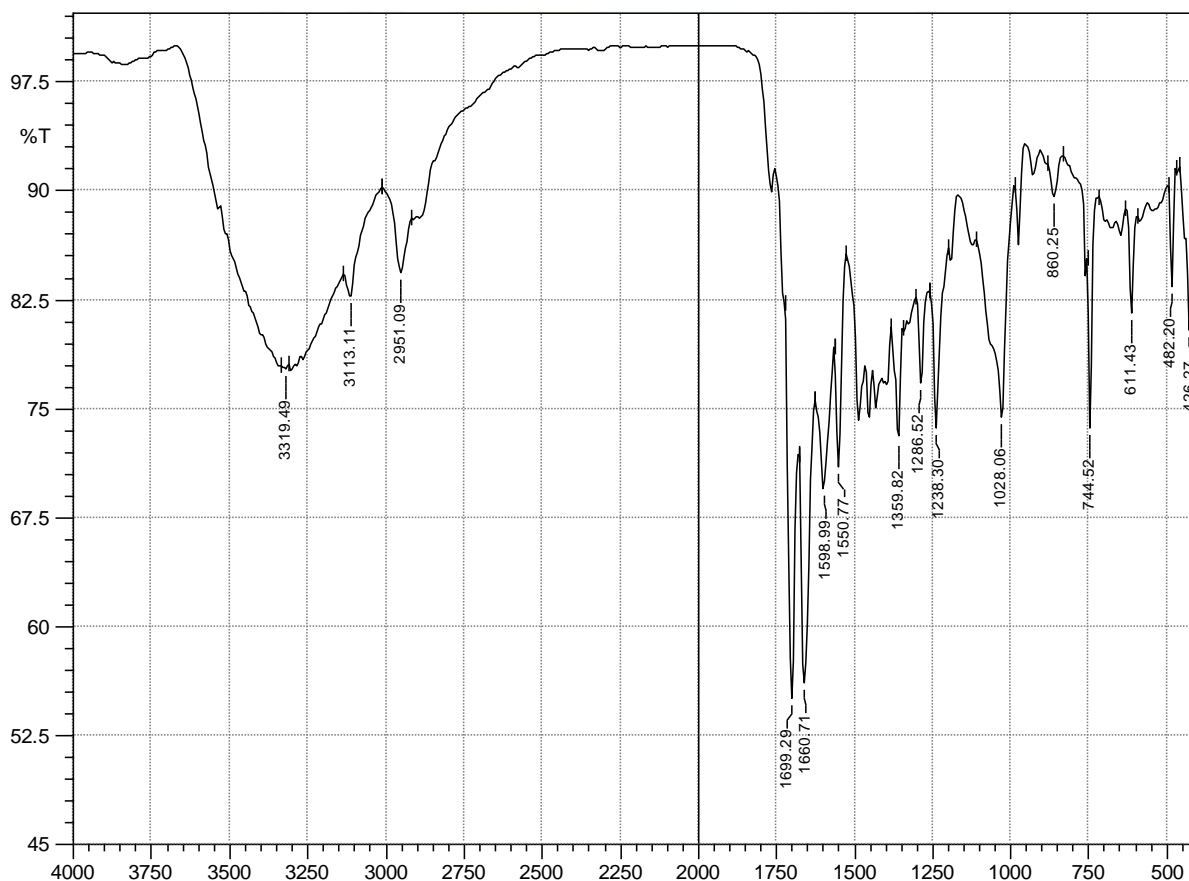


Fig. 3.7

Sample 5: caffeine extracted from roasted coffee bean powder

i. IR spectrum

IR spectrum of the sample extracted from the powdered roasted coffee beans also agrees with the data of standard caffeine sample. The peaks at 2900-3100 cm^{-1} is assigned to C-H stretching absorptions. Strong peaks found at 1699 and 1662 cm^{-1} are due to C=O and C=N stretching absorptions respectively. The C=C bond skeletal vibrations gave IR absorption at $\bar{\nu}$ 1550 cm^{-1} and the strong peak at $\bar{\nu}$ 1238 cm^{-1} is assigned to C-N stretching absorption.

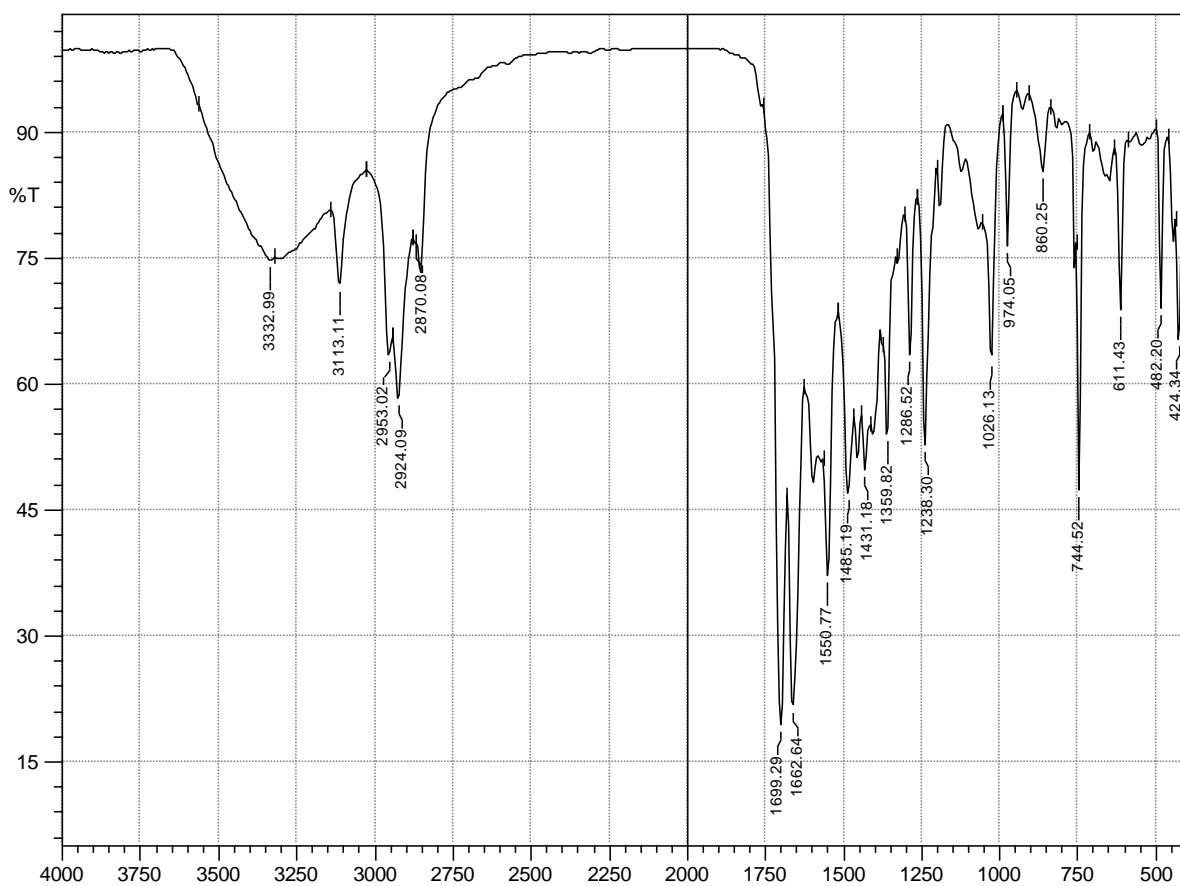


Fig. 3.8

Value of caffeine in the samples analyzed

Table 3.1

Sl. No.	Samples	Caffeine content (in g)	Percentage of caffeine	Melting point observed (in °C)
1	Three Roses Tea	0.2203	1.1015	233.6
2	AVT premium Tea	0.1533	0.7665	233.4

3	Ripple Tea	0.1925	0.9625	233.9
4	Bru Coffee	0.9904	4.952	226
5	Powdered roasted coffee beans	1.4128	7.064	237.5

IR spectral values

Table 3.2

Sl. No.	Samples	$\bar{\nu}$ (C=O) cm ⁻¹	$\bar{\nu}$ (C=N) cm ⁻¹	$\bar{\nu}$ (C=C) cm ⁻¹	$\bar{\nu}$ (C-N) cm ⁻¹	$\bar{\nu}$ (C-H) cm ⁻¹
1.	Three Roses Tea	1699	1662	1548	1238	2900-3000
2.	AVT premium Tea	1699	1660	1548	1238	2900-3000
3.	Ripple Tea	1701	1660	1548	1238	2900-3000
4.	Bru Coffee	1699	1660	1550	1238	2900-3100
5.	Powdered roasted coffee beans	1699	1662	1550	1238	2900-3100

UV-Vis spectral values

Table 3.3

Sl No	Samples	$n \rightarrow \sigma^*$ $\pi \rightarrow \pi^*$ of N-H & C=O	$\pi \rightarrow \pi^*$ of C=O
1	Three Roses Tea	275	237
2	AVT premium Tea	275	241
3	Ripple Tea	275	239

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SUMMARY AND CONCLUSION

Caffeine (1,3,7 – trimethylxanthin- 2,6-dihydroxy purine) constitutes one of the crucial groups of plant alkaloids. It is present in considerable amounts in substances such as cocoa, kola nuts and leaves of tea and coffee plants. Caffeine has pharmacological effects on central nervous system, heart, peripheral and central vasculature, renal, gastrointestinal and respiratory system. Caffeine has been shown to affect mood, stamina, the cerebral vascular system, and gastric and colonic activity. Caffeine is used to restore mental alertness or wakefulness during fatigue or drowsiness. Caffeine is also found in some headache and migraine medications, in certain dietary supplements used for weight loss, and in many popular energy drinks. It has side effects like increase in blood pressure and vasoconstriction. Long term consumption at sufficiently high doses has been associated with chronic arterial stiffness. Coffee and caffeine can affect gastrointestinal motility and gastric acid secretion.

In the present study, we had performed a successive method for the isolation of caffeine from three tea samples and two coffee samples. The percentage of caffeine content in all the five samples were calculated. Among the three tea samples, Three roses has the highest percentage of caffeine value (1.1015). Among the coffee samples, the natural coffee has the highest percentage of caffeine (7.064). The products isolated were confirmed as caffeine by melting point detection and infrared and UV-Visible spectroscopic techniques. The data obtained were in close agreement with the standard sample of caffeine in literature.