PROCEEDINGS OF
GLOBAL CONFERENCE ON
THE CONTROL OF GREENHOUSE GASES AT THE SOURCE BY PHYSICAL AND CHEMICAL TECHNOLOGY

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PROCEEDINGS OF GLOBAL CONFERENCE ON THE CONTROL OF GREENHOUSE GASES AT THE SOURCE BY PHYSICAL AND CHEMICAL TECHNOLOGY

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ENVIRONMENT FOR HUMAN EMPOWERMENT

Prime Minister, Mr. Narendra Modi receives UN's highest environmental honour, "Champion of the Earth Award" from United Nations Secretary General Antonio Guterres at a special ceremony in New Delhi.

Yesterday, the United Nation honoured me with the 'Champions of the Earth Award'. While I was extremely humbled at receiving this honour; I do feel that this award is not for an individual, Instead, It is recognition of the Indian culture and values, which have always placed emphasis on living in harmony with Mother Naturel.

It was a proud moment for every Indian to see India' proactive role in mitigating climate change being acknowledged and appreciated by the United Nations secretary general, Antonio Guterres and Erik Solheim, the executive director of the UNEP.

Human beings and nature have a very special relationship. Mother Nature has nurtured and nourished us. The first civilisations were established on the banks of rivers. Societies that live in harmony with nature flourish and prosper.

Today human society stands at an important crossroads. The path that we take hereon will not only determine our wellbeing but also that of the generations who will inhabit our planet after us. The imbalances between our green and necessities have led to grave ecological imbalances. We can either accept this, go ahead with things as if it is business as usual, or we can take corrective actions.

Three things will determine how we as a society can bring a positive change.

The first is internal consciousness. For that, there is no better place to look than our glorious past. Respect for nature is at the core of India's traditions. The Atharvaveda contains the Prithvi Sukta, which contains unparalleled knowledge about nature and the environment. It is beautifully written in Atharvaveda, "Salutations to Mother Earth. In her are woven together ocean and river waters; in her is contained food which she manifests when ploughed; in her indeed are alive all lives; may she bestow us with that life.

The ancient write about the panch Tatvas-Prithvi(Earth), Vayu(Air), Jal (water), Agni(File), Akash (Sky)-and how our life systems are based on the harmonious functioning of these elements. The elements of nature are manifestations of divinity.

Mahatma Gandhi wrote extensively on the environment and even practised a life-style where compassion towards the environment was essential. He propounded the doctrine of trusteeship, which places the onus on us, the present generation, to ensure that our coming generations inher it a clean planet. He called for sustainable consumption so that the world does not face a resource crunch. Leading lifestyles that are harmonious and sustainable are apart of our ethos. Once we realise how we are flag bearers of a rich tradition,it will automatically have a positive impact on our actions. The second aspect is public awareness. We need to talk, write, debate, discuss and deliberate as much as possible on questions relating to the environment. At the same time, it is vital to encourage research and innovation on subjects relating to the environment. This is when more people will know about the pressing challenges of our times and ways to mitigate them. When we as a society are aware of our strong links with environmental conservation and talk about it regularly, we will automatically be proactive in working towards a sustainable environment. That is why I will put proactiveness as the third facet of bringing a positive change. In this context, I am delighted to state that the 130 crore people of India are proactive and at the forefront of working towards a cleaner and greener environment.

We see this proactiveness in the Swachh Bharat Mission, which is directly linked to a sustainable future. With the blessings of the people of India, over 85 million house-holds now have access to toilets for the first time. Over 400 million Indians no longer have to defecate in the open. Sanitation coverage is up from 39% to 95%. These are landmark efforts in the quest of reducing the strain on our natural surroundings. We see this proactiveness in the success of the Ujjwala Yojana. Which has significantly reduced indoor air pollution due to unhealthy cooking practices that were causing respiratory diseases? Till date, over five crores Ujjwala connection has been distributed, thus ensuring a better and cleaner life for the women and their families.

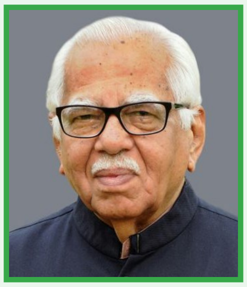
India is moving at a quick pace in cleaning its rivers. The Ganga, which is India’s lifeline, had become polluted in several parts. The Namami Ganga Mission is changing this historical wrong. Emphasis is being given to the proper treatment of sewage. At the core of our urban development initiatives such as AMRUT and the smart cities, Mission is the need to balance urban growth with environmental care. The over 13crore soil health cards distributed to farmers are helping them make informed decisions that will boost their productivity and improve the health of our land, which helps the coming generation. We have integrated objectives of skill India in the environment sector and launched the schemes including Green Skill Development Program for skilling about 7 million youth in the environment, forestry, wildlife and climate change sectors by 2021. This will go a long way creating numerous opportunities for skilled jobs and entrepreneurship in the environment sector.

Our country is devoting unparalleled attention to new and renewable sources of energy. Over the last four years, this sector has become more accessible and affordable. The Ujala Yojana has led to the distribution of nearly 31 crores LED bulbs. The costs of LED bulbs have reduced and so have the electricity bills and emissions. India’s proactiveness is seen internationally. It makes me proud that India remained at the forefront of the COP-21 negotiations in Paris in 2015. In March 2008, world leaders of several countries converged in New Delhi to mark the start of the international Solar Alliance, an endeavour to harness the rich potential of solar energy and bring together all nations that are blessed with solar power. While the world is talking about climate change, the call for climate justice has also reverberated from India. Climate justice is about safeguarding the rights and interests of the poor and marginalised sections of society, who are often the menace of climate change.

As I have written earlier, our actions today will have an impact on human civilization much beyond our time. It is up to us to take on the mantle of global responsibility towards a sustainable future. The world needs to shift to a paradigm of environmental philosophy that is anchored in environmental consciousness rather than merely government regulations. I would like to compliment all those individuals and organizations who are working assiduously in this direction. They have become the harbingers of a monumental change in our society. I assure them all possible support from the government in their pursuits. Together, we will create a clean environment that will be the cornerstone of human empowerment.

Narendra Modi

Ram Naik
Governor, Uttar Pradesh



No.468 /PS-GOV

Raj Bhavan
Lucknow - 226 027

18 March, 2019

Dear Prof. Kaman Singhjee,

Subject : Invitation as Chief Guest at 'Global Conference on Control of Green House Gases at the Source by Physical and Chemical Technology'

Please refer to your letter dated 09.03.2019 inviting me as Chief Guest at 'Global Conference on Control of Green House Gases at the Source by Physical and Chemical Technology' organised by Department of Chemistry, School of Physical and Decision Science (SPDS), Babasaheb Bhimrao Ambedkar University, Lucknow on 22 April, 2019.

Due to preoccupation it will not be possible for me to attend the Conference. I extend my Good wishes for the success of the programme.

With regards,

Yours sincerely

(Ram Naik)

Prof. Kaman Singh,
Chairman/Convener,
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GCGHGSPCT-2k19
GLOBAL CONFERENCE ON THE CONTROL OF GREENHOUSE GASES
AT THE SOURCE BY PHYSICAL AND CHEMICAL TECHNOLOGY

Ref. : GCGHGSPCT 2K19| PM| INVITATION/BBAU **Date :** 28/11/2018

November 28, 2018
Sh. Narendra Modi
Honourable Prime Minister
South Block Raisina Hill
New Delhi-110011 (India)
FAX No. 011-23012312

Global Conference on the Control of Green House Gases at the Source by Physical and Chemical Technology (GCCGHGSPCT2k19)

Sir,

The event has been proposed on the **World Earth Day- April 22, 2019**, by the Department of Chemistry, School of Physical and Decision Sciences (SPDS), Babasaheb Bhimrao Ambedkar University (A Central University), Lucknow, U. P., India

Venue: Bharat Ratna, Atal Bihari Bajpai Auditorium BBAU, Lucknow

The objective of this Global Conference is to motivate the people particularly the younger generations, that a long-term permanent solution of the Global protection of environment caused by air pollution is possible if we can arrest Green House Gases right from the sources and do not allow Green House Gases to escape to the atmosphere.
While celebrating the World Earth Day, we pledge to spread the knowledge and methodical understanding of the experts from India and abroad. This will encourage teamwork along with the transfer of vast knowledge in all fields of Environmental Pollution, Remediation, Ecological issues including Global warming, wastewater treatment, Green chemical technology, and related matters.

The world is witnessed to your personal example of spectacular feat, strategic leadership & relentless pursuit while addressing the issue of climatic change pioneered by you in our illustrious country Rightfully so, an apt recognition- '**Champions of the Earth Award**' – the highest UN Honour for Environment was conferred upon you by the UN Secretary General Antonio Guterres. We are sanguine that an ambitious & popular leader like you will propel us forward in the fight to keep the natural environment healthy, accessible and sustainable for all. While the entire country is following your footsteps, we in our Academic Fraternity –with our Scholars & Students in particular are infused with tremendous alacrity, inspiration & motivation to contribute in our humble way to make your Mission successful. We, therefore are committed to bring out the best research undertaken by Experts – both from India & abroad during the International Conference in the Field of Controlling Green House Gases with the sole aim to suggest measures for making the entire world a better place to live in.
Therefore, we take this opportunity to invite you on the occasions of Earth Day and this Conference to guide and bless us for the beginning of a new approach to control air pollution to the environment.

With high respectful regards;

Kaman Singh
Chairman/Convenor

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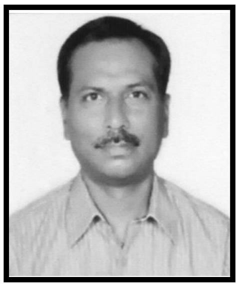

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Department of Chemistry, BBAU, Lucknow

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Department of Chemistry, BBAU, Lucknow

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PLENARY SPEAKER-01

A Radical Approach to Control Global Warming & Air Pollution in Cities

Professor Mahendra Prasad
Former Director
National Sugar Institute, Kanpur, INDIA
Now @ Simon Fraser University, Burnaby B C, CANADA

Global warming and air pollution caused by the emission of green house gases produced by transportation, thermal power plants and industries, experienced in recent years are severe. It is anticipated that by the end this century earth's environment temperature would be increased by 6^0 Celsius. Such increase in temperature will have dangerous impact on healthy life of people on this planet. Therefore, we need to work out and formulate guidelines not only for reduction of formation of green house gases in all sectors rather a real sustainable approach to eliminate the impact of these gases that cause global warming be initiated. In this deliberation it is proposed to arrest green house gases at the source in the transport system and to convert them into useful commercial products for the utilisation of by common people. Success gained in this approach will suggest the future guidelines to control global warming and air pollution in the cities.

PLENARY SPEAKER-02

India's Climate Action for a Sustainable World

Dr. Srikanta K. Panigrahi
Director General
Indian Institute of Sustainable Development (IISD)

PLENARY SPEAKER-03

Environmental Pollution Greenness and Heart Diseases

Prof. Sanjay Srivastva
University of Louisville, USA

PLENARY SPEAKER-04

Green House Gas Control using Nuclear Technologies

P. S. Dhami
Fuel Reprocessing Division, Nuclear Recycle Group
Bhabha Atomic Research Centre, Trombay, Mumbai-400085
Email: psdhami@barc.gov.in

With the advancements in science and technology, the quality of air we breathe and the environment around us is changing gradually, creating several challenges, including global warming to our planet. Therefore, to keep our planet safe, environmental friendly processes and technologies have to be employed for powering our homes, workplaces and cities. Ongoing demand for electricity in the entire world is presently met by the combustion of fossil fuels like oil, natural gas and coal. During the combustion process, several pollutants such as fly ash (containing diverse trace elements (heavy metals)), CO_2, SO_x (SO_2 and SO_3), NO_x (NO, NO_2), Hg, and VOCs are released into the atmosphere that affect human health, crops and forests besides increasing corrosion.

The electron beam generated from accelerators is found to be a superior multi component air pollution control technology when compared to conventional ones for treatment of flue gases as they produce less secondary waste besides producing high-quality fertilizers as by-products. Additionally, volatile organic compounds (VOCs) can also be degraded using beam technology.

To meet energy demand, alternate sources are being explored globally. Among the several sources, nuclear energy is being projected to be one of the most cost-effective, long lasting and clean energy source. As relatively low carbon dioxide is emitted, its contribution to the global warming is therefore relatively low. It is now generally agreed that the world must rapidly reduce CO_2 emissions, the largest contributor to the green house gases, in order to fight off dangerous climatic changes, but how? This remains the topic of the debate.

For long-term nuclear power production India has adopted a three stage nuclear programme. Among the two fuel cycle options we follow closed fuel cycle option for spent fuel management. The proven resources of low priced uranium are insufficient to support the long-term and meaningful contribution to India's energy demand by way of nuclear energy. Closing the nuclear fuel cycle by reprocessing the spent fuel and recycle of uranium and plutonium back into reactor systems helps in exploiting the full potential of nuclear power and maximizes the resource utilization. In nuclear fuel cycle, green chemistry is currently followed at back end of nuclear fuel cycle. A brief account on recycling, reuse and recovery of useful radionuclides for societal applications will be presented in this plenary talk.

PLENARY SPEAKER-05

Climate Change and Global Warming: Exploring New Solutions using EA^2 Approach

Pradeep K. Srivastava
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Medicinal & Process Chemistry Division, CSIR-Central Drug Research Institute,
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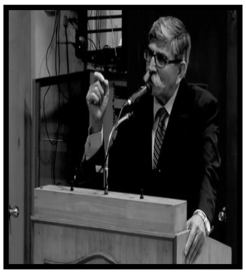
Sometimes back the president of Maldives informed the media that he wants to buy land for his country. People were surprised on this statement as why to buy such vast land? The answer is very simple as Maldives is in the hit list of global warming and is only an average of two meters above the sea level. Any future change in the climatic condition will make sea level to rise affecting many countries in the world including Maldives. The first country in the world which will be soon submerged in the ocean is Tuvalu which is in Pacific Ocean and people of that country are already fleeing to neighbouring countries. More than 1 Crore 50 lakhs acres of land is converted into desert every year in the world. This has caused global warming and also made 10 crore people to become homeless. The major reason for this is increasing green house gases in the atmosphere and deforestation. Coral reefs are unique ecosystems of plants, animals, and their associated geological framework. The ocean equivalent of rainforests, they are home to 25% of all marine species, yet it is estimated that many of the world's reefs will be destroyed or significantly damaged in the next 20 years. There are about 4,000 coral reef fish species worldwide, accounting for approximately a quarter of all marine fish species. The Great Barrier Reef, measuring 2,000 Kms. in length, is the largest living structure on Earth. It can be seen from the Moon. Reefs protect human populations along coastlines from wave and storm damage by serving as buffers between oceans and near-shore communities. Nearly 60 per cent of the world's remaining reefs are at significant risk of being lost in the next three decades. The major causes of coral reef decline are coastal development, sedimentation, destructive fishing practices, pollution, tourism and global warming. Climate change threatens to destroy the majority of the world's coral reefs, as well as wreak havoc on the fragile economies of Small Island Developing States. Two hundred drug-yielding plants have become extinct by the end of the last century and the loss of each plant had been worth around more than $ 203 million. It's an alarming news as drugs obtained from the plants are more effective, well tolerated and less toxic. Plants provide us a number of drugs starting from morphine to taxol and a great future lies ahead in plants from marine sources, which can provide us especially newer antibiotics. Environmental factors like global warming caused by chlorofluorocarbons, per fluorocarbons, UV radiation besides deforestation, desert formation and industrial pollution may cause extinction of several medicinal plants even before their medicinal value is known to us. In India, northeast areas and Western Ghats region are already among the mega biodiversity rich areas of the world. Northeast region of India has a special kind of vegetation which has at one hand Himalayan impact and on the other hand has got the coastal impact due to the nearby Bay of Bengal.

We need to reach to not only the conservation experts or scientists but will have to explore and to learn from the traditional knowledge at one point and using the latest technologies like BIONICS or BIONIC ENGINEERING at other point to combat this global issue of climate change and increasing green house gases. This paper will focus on the effective use of a new science called Scientoonics which uses a novel concept of ***scientoons*** developed by the author for the first time in the world coupled with **EA^2 approach** (EA^2 is called Awareness, education and finally the action) in planning the unique strategy from saving us from Global warming especially for Asia and Pacific region.

PLENARY SPEAKER-06

Water: Need for the Conservation for the Nation Building



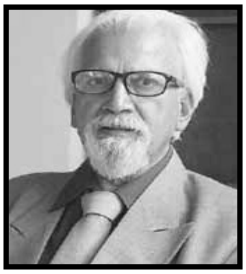
Major General Ajay Kumar Chaturvedi
AVSM, VSM

Extract: Water is the excelsior of life. However fresh water is depleting world over at an alarming rate. Population explosion, global warming, deforestation, pollution are some of the important reasons for emerging crisis. Situation in India and for that matter in the entire South Asia is further getting aggravated due to a host of local reasons. Most of the rivers in North and East of India are glacier fed and the topography of glaciers in this part of the world is such that not only they are melting faster than normal but they also bring lots of silt with them, accumulation of that is making rivers shallower than normal which is firstly resulting into floods and secondly making the existing water resorvoirs highly inefficient . Water storage capacity in India is as it is less than the world average and that leads to lots of rain water getting drained into the sea without its useful utilisation. Unchecked draining of industrial effluents and untreated sewage finding its way into the water channels, social and religious apathy resulting into non decayeable waste making water unusable, shifting to water intensive crops in recent times and not sharing the legitimate share of water by the Upper Riparian (China) with the lower riparian (India) are adversely affecting the available surface water. To further add to the water woes it is now clearly established that the depleting water table is making the ground water also contaminated due to typical soil chemistry of the river basins of Northern and Eastern India, namely; Indo Gangetic Basin, Indus River Basin and Ganga Brahmaputra-Meghna Basin. Finiteness of fresh potable water available in the nature makes it obligatory on the part of the government and the people to devise ways and means to conserve the available fresh water, try to enhance water availability, build infrastructure of water storage , go for minimising water utilisation and finally come out with engineering/technology based water utilisation practices for utilisation of treated water.

Keywords: Conservation, collective responsibility.

PLENARY SPEAKER-07

Carbon Dioxide Miraculous Gas



Dr. Ram Lakhan Singh
Indian Forest Service (Rtd.)

1-Carbon dioxisde though has been grouped with the Green House Gases (GHG), but its other properties making a miraculous gas.

2-It performs the key role on liberating the oxygen from the carbon and hydrogen as may be seen in the Assimilation Equation, of the Photosynthesis operation performed by the green plants.

6co2+6r2o+675 kilocalory solar energy+c6h1206+o6

3-The 21 percent of the volume of the earth's atmosphere is occupied by oxygen and all of it is the product of the carbon dioxide. The carbohydrate produced in the proses is nothing but the timber, flowers, leaves, food etc. The timber and other tree products are solidified CO2. India is importing large amount of tree products. It means we are purchasing solidified CO2 from other countries. Whereas we can easily grow but we are not able to do so because of low priority of the planting tree. We have to learn from trees how they combine CO2, and water (H2O) and use solar energy to release oxygen and manufacture Carbohydrate. Trees now it we don't.

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DISTINGUISHED SPEAKERS (DS)

DS-01

Greenhouse Gases Challenge–Chemical Science Solution

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It is well recognized fact that excessive release of greenhouse gases (GHGs) in the atmosphere owing to escalated human and industrial activities, adversely impact the Earth's environment. This results in global warming, damage to protective ozone layer, degradation of ecosystems and depletion of natural resources. Unabated, GHGs severely burden economies and societies and jeopardize the very existence of life on Earth. Control of GHGs and mitigation of their ill-effects is imperative to move to a path of sustainability and the security and development of humankind. The chemical and physical sciences can and must play a key role in developing processes, products and monitoring mechanisms and provide sustainable solution for tackling many of the emergent challenges due to GHGs.

Chemical science with its endless frontiers can provide sustainable solution for tackling many of the problems related to GHGs. It can play central role in developing a scientific understanding of the climate system and consequences of climate change, improving our understanding of atmospheric and ocean chemistry and biology, develop new energy and carbon mitigation solutions, help crops and flora and fauna to tolerate the changing conditions, etc.

This presentation would uncover as to how chemical science offers great opportunities for addressing the emergent global challenges related to Earth's climate through advancement of green and sustainable chemistry and chemical technologies, particularly with regard to providing clean energy alternatives and development of chemical and chemical products through safer and sustainable means of utilizing bio-privileged molecules. The talk would accentuate on highlighting the essentiality of upgraded and amplified education and research with focus on developing chemical understanding of climate system, GHGs challenges and green chemical technologies for various purposes.

DS-02

Status of Environment in South Asian Region: In Reference to Prosperity

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Over the past few decades, it has been claimed that a large volume of works have been carried for the prosperity of the people living in South Asian region. This region is famous for its unparalleled geographic features in the form of snowcapped mountains, hills, plains, deserts, biodiversity especially in water resources. It is natural to expect the prosperity of the people of countries of this region. The rapid industrialization and urbanization have put the pressure on environment and depleted the natural resources. In spite of being rich in natural resources and exploiting them quality of life of the people is not up to the mark. Public health condition is not good due to lack of proper sanitation, lack of nutritious diet in their meal and lack of safe drinking water. Till now the new areas of knowledge and investigations continues but mostly confined to laboratories and been matter of academic discussion among specific scientific community remaining aloof from the common people. Therefore, further progressive steps must be taken to take modern research out of the laboratory and reveal relevance and utility of science to uplift the life of common people. Moreover, the logic and the ideas based on the observation, research works, direct contact to the common people and field visit and empirical evidences to envisage a progressive and pro-people perspective for ecology and development policy debate of the region. Main features of environmental problems and related challenges are wrong urbanization and induced pollution, environmental issues liked with rural livelihood, pursued wrong infrastructure and development model, rapacious nature against the environment and global change and natural disaster. Another important issue is food safety which demands an integrated response from the way it is grown or raised to how it is collected, processed, packaged, sold and consumed. This is directly related with public health which is questionable from the social justice view point. Significant number of poor people live in South Asian region, is matter of unpleasant. It is clear that reckless exploitation of resources will only find way to plunder more resources and accumulate more wealth. Making money at the cost of environment is present day problem which affects the whole region. Therefore, scientific community must come forward for sustainable development with the aim of social justice. Our science education should be productive in order to have sustainable livelihood with good human norms and values. Only the pro-people scientific approach to address the problem could lead the entire region towards prosperity.

Keywords: South Asian Region, Environment, prosperity, Livelihood, Public Health, Disaster

DS-03

Green House Effect, Global Warming and Ozone Depletion–Causes, Consequences and Remedial Measures

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The earth's atmosphere works like a glass greenhouse where plants are kept. When the sun's rays enter our atmosphere, most of it continues right down to the earth's surface. When they hit the soil and surface water, they release most of their energy in the form of heat. Some of the heat then radiates back out into space. However, there are certain gases like carbon dioxide and methane that absorbs heat and radiate it back to the earth's surface. This helps to keep our atmosphere warm. These gases are therefore called greenhouse gases because of their heat trapping ability. As a result, the temperature of the Earth's surface starts rising which leads to Global warming. This effect of trapping higher wave length Infra Red (IR) radiations and then reinforcing the solar heat is known as "Greenhouse effect". There are several greenhouse gases emitted by humans in a variety of ways and it is these greenhouse gases that are responsible for climate change. The gas that is responsible the most for global warming is carbon dioxide. The other gases responsible for this phenomenon include methane and nitrous oxide. These gases vary from each other in their heat trapping abilities and nitrous oxide is said to be the most powerful heat trapping gas. Even chlorofluorocarbons released from air conditioners and refrigerators have a much greater heat trapping potential than carbon dioxide.

The temperature of the earth is rising rapidly. It has been estimated that this rise has been about twice the rate it was about 50 years ago. Scientists believe that the main reason behind this sudden rise is the effect of greenhouse gases emitted by various human activities such as deforestation, burning of fossil fuels and fire woods, cement industries, forest fires, etc. Burning of fossil fuels has significantly increased the concentration of carbon dioxide in the atmosphere. It has been estimated that the current concentration of carbon dioxide in the atmosphere is about 30 percent greater than it was 6,50,000 years ago. As a result, the temperature of the earth has increased drastically and natural calamities like droughts and floods are becoming more and more common. It is estimated that the global temperature would rise by 1°C to 5.8°C by 2100 at the current rate of warming. Scientists have predicted that the world would be warmer by more than half a degree in next 20 years, if CO_2 emissions are not reduced.

The ozone that is present in the upper layer of the atmosphere, about 40 km from earth surface, is known as the "ozone layer". This layer protects life on earth by absorbing most of the ultraviolet radiation that is emitted by the sun. It prevents UV C and part of UV B to reach the Earth's surface. When man-made chlorofluorocarbons (stable for 20-120 years) reach the ozone layer, they are broken apart by short-wave energy from the sun. The free chlorine atoms then break apart the molecules of ozone, thus creating holes in the ozone layer (Antarctica).

Hence, ozone layer depletion causes exposure to too much of ultraviolet radiation leading to skin cancers (such as Squamous cell carcinoma (SCC), Basal cell carcinoma (BCC), Malignant melanoma (MM), Non malignant melanoma (NMM), suppression of the immune system, cataract, erythema and edema. It is also believed to reduce the productivity of certain crops.

Global warming has resulted in a series of devastating climate disasters and extreme weather events such as hurricanes, heat waves and floods. Millions of homes throughout the world are now either underwater or have been blown away. The increase in air and water temperatures has lead to rising sea levels, higher wind speeds, prolonged droughts and heavier precipitation. More than 150 million people live in coastal areas that will be below the sea level by the end of the century and are under threat of getting marooned.

My lecture will deal on various aspects of Green house effect, Global warming and ozone depletion- causes, consequences and remedial measures.

DS-04

Methane (CH_4) as a Potent Green House Gas: Its Sources and Sinks

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Methane (CH_4), a potent greenhouse gas (GHG) contributing about one third to the global GHG budget, owing to the ecological and anthropogenic perturbations. The CH_4 absorbs IR radiation as a result enhances the Earth's temperature ~15 to 20%. The CH_4 is produced from natural (termites, oceans, enteric fermentation, etc.) and anthropogenic sources (paddy cultivation, coal mining, biomass burning, etc.) globally. Mostly, anthropogenic activities are accountable for the key fraction (~566 Tg CH_4/year) of global CH_4 emissions. However, natural sources also add (208 Tg CH_4/year) significant amount of CH_4 into the atmosphere. The CH_4 is emanated by human interference through several sources i.e. paddy cultivation, agricultural livestock, hydrocarbon excavation, coal mining, landfill practices and biomass burning, etc. In addition, the natural sources include wetlands, lakes, estuaries, oceans, gas hydrates, terrestrial plants, wildfires and permafrost, etc. In water logged (paddy fields) and swampy areas, CH_4 is generated by anaerobic CH_4 producing (methanogens) *Archaebacteria*. The CH_4 is oxidized in nature adapting both chemical and biological courses. The key consumers of CH_4 are photochemical oxidation (~90%) in troposphere and stratosphere by free OH^- radicals 'the detergents of the atmosphere'. While CH_4 consuming bacteria (methanotrophs) consume about 6-10% of CH_4 globally. Methanotrophs (also known as CH_4-oxidizing bacteria) are the only CH_4 consuming biological source in upland soil, mitigating the problem of CH_4 due to the presence of unique CH_4 oxidizing enzyme CH_4-monooxygenase. The paddy agriculture land expansion and urbanization activities across the globe are leading to the removal of forest cover consequently increasing of GHGs load. The gradual conversion of forest into agro- ecosystem reduces the CH_4 consumption potential of methanotrophs in soil. Therefore, afforestation, land use management and improved dry land paddy cultivation strategies may significantly contribute in minimizing the CH_4 emissions.

Keywords: CH_4, GHG, Global Warming, Climate Change, Methanogens, Methanotrophs

DS-05

Wind Energy and Solar Energy as Alternate Energy Sources with Particular Reference to India

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Wind energy is the kinetic energy associated with the movement of atmospheric air and this energy is converted to more useful forms of power using wind energy systems. It has been used for hundreds of years for sailing, grinding grain and it is being used to generate electric power. Windmills for water pumping have been installed in many countries particularly in the rural areas. The power generation projects contribute to the socio-economic development of the country.

India is now recognized as a leading country in the world in the development and utilization of renewable energy, in general and in the development of wind power, in particular. Along with the growth in the Indian economy energy consumption is also increasing to meet the growing demands of the industries. Power generation from renewable energy sources has assumed significance in the context of environmental hazards posed by the excessive use of fossil fuels. Exploiting an alternate source of energy is the need of the day in view of the increased power demand and depletion of conventional energy resources such as fossil fuel. Also, wind energy generation will save valuable foreign exchange, which otherwise is being used for importing oil for power generation by conventional resources.

Another type of non-conventional energy that can be made available is solar energy. Solar heat can also be used to generate electricity. Solar energy has applications in many devices that convert solar energy directly into electricity Solar thermal energy is being used in India for heating water for both industrial and domestic purposes. In this presentation an attempt has been made to project and discuss the current scenario prevailing in our country regarding the use of these two types of energy.

Keywords: Wind Energy, Solar Energy, Wind Mills

DS-06

Fabrication of Cost Effective Polymer Screen Printed Solar Cells

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A Solar cell is a device that converts the light energy into electrical energy by the photovoltaic effect. Traditionally the solar cells were made from silicon or glass substrate. However there are some problems are associated with traditional solar cell like high overall cost, less portability and durability etc. As a technology polymer solar cells are only photovoltaic technology that potentially offers a convincing solution to the problem of high overall cost commonly encountered for other photovoltaic technologies. Polymer solar cells offer production in high volume at low process cost. Recently, the research on the polymer material for solar cell has been focussed mainly on improving the power conversion efficiency for small laboratory cells. Also, on the module level, various commercially available polymers are used for encapsulation and other encasing purpose of the solar module. In this paper the fabrication of a complete polymer solar cell module is shown in the normal room conditions. A typical screen printing method is applied to print solution on a flexible substrate. Various types chemicals such as Ag paste, ZnO, ITO etc are screen printed and dried layer by layer. For physical strength encapsulation is done mechanically by PET and subsequently polymer junction box is developed and fitted. A mass production of solar module technology is investigated on local level. This production technique is scalable and can be adapted by the industry. The experimental work shows some potential outcomes to select the screen printing technique for fabrication of polymer solar cell.

DS-07

Atmospheric Burden of CO_2 and Non-CO_2 Greenhouse Gases and Climate Change

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Increase in greenhouse gases concentration in the atmosphere has produced a larger global mean warming than has been observed in the past. As a result of anthropogenic emissions of greenhouse gases particularly carbon dioxide (CO_2) from fossil fuel combustion the Earth's climate is warming. Based on stability test of Vector Auto Regressive (VAR) model, we have used the impulse response functions and the variance decomposition method for the analysis of climate variability. We have examined the possible connections among the atmospheric abundance of CO_2 and some climate indicators, viz., the global temperature anomaly, the global mean sea level, the global sea-ice extent and the global precipitation anomaly occurred during last forty years (1978-2017). We have studied the effect of CO_2 as anthropogenic forcing for the next decade. We have observed that the global temperature in the next decade will increase by 2.7%; mean sea level will increase by 6.4%. Increasing abundance in CO_2 will be responsible for about 0.43% decrease in the sea-ice extent while there will not be any change in the precipitation pattern. Anthropogenic emissions of non-CO_2 greenhouse gases, such as ozone-depleting substances (largely from sources other than fossil fuels), also contribute significantly to warming. Some non-CO_2 greenhouse gases have much shorter lifetimes than CO_2, so reducing their emissions offers an additional opportunity to lessen future climate change. Although it is clear that sustainably reducing the warming influence of greenhouse gases will be possible only with substantial cuts in emissions of CO_2, reducing non-CO_2 greenhouse gas emissions would be a relatively quick way of contributing to this goal. To that end, we also have analysed 52 years (1965–2017) data of the ozone depleting substances using the Box-Jenkins model and have predicted the future trend of the ODSs until the year 2030.

DS-08

Global Warming and Climate Change: Interactions, Toxicity to Remediation

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The global warming is a well known process which occurs when gases in earth's atmosphere trap the sun heat and has significant effect on climate and us as inhabitants. Several factors are responsible for global warming including transportation, modern lifestyle, overexploitation of natural resources etc. Globally, the energy consumption is exponentially increasing due to population and our quest for a higher living standard and these environmental changes poses emerging environmental health challenges.

The risk of pollutants may change in future due to alteration in degrees of direct and indirect exposure patterns, fate of chemicals [POPs, PCBs, Methyl mercury, chloromethane] and thus strategic management practices are needed. Few chemicals viz Bisphenol A, phthalate, styrene etc from plastic may accumulate and impair organ function. Waste management practices- landfills, recycling without adequate safety measures, incineration emit greenhouse and toxic gases which are released into the atmosphere, soil and waterways, contributing to the increase of the greenhouse effect. Exposure to UV-B radiation may decrease the toxicity of some pollutants e.g methyl mercury, due to its role in demethylation but increase the toxicity of other pollutants such as some pesticides and polycyclic aromatic hydrocarbons. Feeding on microplastics by zooplankton may lead to bioaccumulation in fish. They are found in up to 20% of fish marketed, potentially threatening food security. Depletion of stratospheric ozone has altered climate in the southern hemisphere in ways that have increased oceanic productivity and consequently the growth, survival and reproduction of many sea birds and mammals. The toxicological profiles of chloromethane and health effects have been investigated and have been classified as probable carcinogens. Innovative methods are essential to combat adverse implications of toxicants or minimize the impacts on aquatic ecosystems. As per Intergovernmental Panel on Climate Change, quantification of the influences on the global climate is complex and many regional effects remain uncertain.

We need to expand the use of renewable energy and transform to cleaner energy system for safer future generations. We must place limits on the amount of carbon emissions, build clean energy economy, reduce deforestation. The advanced technological solution aims to improve carbon sequestration through geo-engineering and Bioinnovation with reduction of carbon footprints. We need to understand the risk on marine ecosystems, sea foods and chemical interactions with anthropogenic organic pollutants.

Keywords: Climate Change, Impacts, Toxicity, Waste Management, Microplastics, Remediation

DS-09

Climate Agreement, Green House Gas Emissions: Issues and Possibilities for Developing World

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On a historic occasion where nearly 200 countries agreed on the deal in Paris last December at the 21⍰⍰ session of the Conference of the Parties to the United Nations Convention (COP21). It agreed on a long-term goal of keeping the increase in global average temperature to much below 2°C above pre-industrial levels, by bringing down the greenhouse gas emissions. Global carbon emissions from fossil fuels have significantly increased since 1900. Since 1970, CO_2 emissions have increased by about 90%, with emissions from fossil fuel combustion and industrial processes contributing about 78% of the total greenhouse gas emissions increase from 1970 to 2011. Agriculture, deforestation and other land-use changes have been the second-largest contributors. Emissions of non-CO_2 greenhouse gases have also increased significantly since 1900.

It also aims to limit the increase to 1.5°C, since it would significantly reduce the risks and impacts of climate change. According to the terms of reference, the agreement will not be binding until at least 55 countries accounting for at least an estimated 55% of the total global greenhouse gas emissions ratify it. With European Union and India joining the ratification now it is less than a few days from now the Paris agreement on Climate Change comes into force. These events are not only milestones but intriguing too for many of us shall be discussed all over for quite some time. While India ratified the Paris agreement on climate change which the world's fourth-largest carbon emitter is accounting for 4.1% of the total global emission, is the 62nd nation to ratify the agreement. After India's ratification, the total emission share of the countries has reached the 51.89%

mark. If you compare with European Union who too is a recent ratifier, accounting for 12.1% of the total global emission, thus the climate deal enters into force this November.

India's commitment to the agreement stands that having signed the agreement, India plans to reduce its carbon emission intensity, i.e. the emission per unit of GDP, by 33-35% from what it was in 2005, by 2030. The main aim is to produce 40% of the total electricity from sources other than fossil fuels. This would mark a significant shift from the coal-based power generation to alternative renewable energy sources. Solar photovoltaic panels, along with large wind mills will contribute to the production of the electricity as per the plan. This could spell a huge opportunity for banks and global companies to enter the sector and make investments. As much as 100 GW of electricity is to be generated from solar energy, of which 40 GW would be through individual rooftop systems. India also envisages employing other renewable energy sources like biomass energy and hydropower.

India propose increase its forest cover by five million hectares along with an improvement in the quality of green cover of an equal measure to create an additional carbon sink of about 2.5 billion – 3 billion tonnes by 2030.A carbon sink is a system that is capable of absorbing carbon dioxide (CO2) from the atmosphere. Currently, over 24 per cent of India's geographical area is under forest and tree cover, which needs to be increased to 33 per cent. While it's a herculean task and a lot will need to be done to achieve the target, we can say that a beginning has been made.

Keywords: Climate Change, Green House Gases, Carbon Emission, Paris Agreement, Ratification

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DS-10

Versatility of Carbon Dioxide: Renewable Applications & Synthetic Explorations

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The production of carbon dioxide around the globe resulting the emergence of global warming day by day. Burning of coal, vehicles fuel, natural gas and nuclear explosions also generates carbon dioxide in the environment, has been the major constituents which majorly influences the global warming. This burden of carbon dioxide in our environment necessitates the need of transforming carbon dioxide into greener valuable products. Also, carbon dioxide has been playing an important role in balancing our environment through photosynthesis in plants.

In recent years, carbon dioxide has been employed as a cheap and safe alternative eliminating the use of harmful reagents such as CO and $COCl_2$. Recently, carbon dioxide has frequently been employed as a green reagent in its various conditions and forms for the syntheses of structurally diverse biologically potent scaffolds employing diversity of starting materials, reagents and catalytic systems. In the present talk, I will focus some of the greener applications of carbon dioxide as a source of renewable energy & its synthetic utility.

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INVITED TALKS (IT)

IT-01

Bio-Fuels: Need of the Hour

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Rudolph Diesel, 1912 had said: "The use of vegetable oils for engine fuels may seem insignificant today, but such oils may become in the course of time as important as the petroleum and coal tar products of the present time." and when Henry Ford, 1925 said: "The fuel of the future is going to come from fruits, potatoes, weeds, sawdust - almost anything. that can be fermented. He even made a car which was running on fuel Ethanol in 1908. Petroleum was cheap and in abundant so it started being used as a fuel. But this has created a damage and badly polluted the environment. The answer to this is Bio-Fuels.

The Earth is passing through a very difficult phase of global warming with the CO_2 levels having shot up from 280 ppm in 1960 to more than 400 ppm now (DANGEROUS LEVELS BEYON 450PPM). In ice age it was 180 ppm. The temperature risen by more than 1.4 F (0.8 C) leading to problems related to Tsunami, floods, melting glaciers and erratic seasons. Anthropogenic emissions contribute to global warming by burning fossil fuels such as coal, petroleum diesel and above all deforestation in the name of development, for forests are great carbon sinks. We have reached a stage where the use of fossil fuels are totally stopped and renewable fuels such as Bio-fuels such as Bio-Diesel and Bio – Ethanol which are" solar liquids" are promoted. and are the need of the hour. They are going to play an extremely important role in addressing global warming concerns associated with petroleum fuels. But also in meeting India's energy needs, which are expected to grow at 4.8% over the next couple of decades and will address energy security as we presently import 75% of the total crude costing 7 lac crore/year and also

Diesel is highly polluting and carcinogenic and its demand is five times petrol. So its very pertinent that it be replaced. Ethanol and bio diesel are gaining world wide acceptance as bio fuels, ethanol in spark-ignition engines and bio-diesel in compression-ignition engine vehicles which up to 15-20% blending need no change in engine. Other fuels are Dimethyl ether (DME) or blends with diesel for buses trucks as clean fluids by volvos in Japan, Europe, USA and Fischer-Tropsch liquids (FTL) made from Coal used in South Africa as diesel. Nitin Gatkari, Transport Minister says blending of Bio- ethanol will go up to 22.5% and of bio-diesel upto 15%. As ethanol produced from molasses is not sufficient to meet the blending even up to 10% Thus, the second generation fuel from the lignocellulosic biomass like bagasse wood etc needs to be tapped.

In our laboratory both Bio-Ethanol and Bio-Diesel are being synthesized. Bio-Ethanol has been produced from Corn Cob and Bio-Diesel by the effect of Oleaginous microorganisms including bacteria, mold, yeast, microalgae effect on Bagasse to produce lipids and their further transesterification to produce Bio-Diesel. For Ethanol the bioconversion was carried out using hybrid approach for co-utilization of dilute acid hydrolysate (pentose rich stream) and hexose rich stream obtained by enzymatic saccharification employing commerciial Cellac – Ctec2 as well as in-house cellulase preparations derived from *Malbranchea cinnamomea, Scytalidium thermophilium* and a recombinant *Aspergillus* strain. Foe Ethanol, Acid hydrolysis (1% H_2SO_4) of corncob at 1:15 solid liquid ratio led to removal of 80.5% of hemicellulosic fraction. The solid glucan rich fraction (63.5% glucan, 8.3% pentosans and 27.9% lignin) was hydrolysed at 10% substrate loading rate with different enzymes for 72 h at 50 °C resulting in release of 732 and 535 (mg/g substrate) total sugars by Cellic CTec2 and *M. cinnamomea* derived enzymes, respectively. The fermentation of enzyme hydrolysate with co-culture of *Saccharomyces cerevisiae* and *Pichia stipitis* added in sequential manner resulted in 3.42 and 2.50% (v/v) ethanol in hydrolysate obtained from commercial Cellic CTec2 and *M. cinnamomea*, respectively. Employing a hybrid approach, where dilute acid hydrolysate stream was added to solid residue along with enzyme Cellic CTec2 during staggered simultaneous saccharification and fermentation at substrate loading rate of 15% resulted in 252 g ethanol/kg corncob. By this method glucose produced was immediately fermented and less inhibitors were produced making the process more efficient and quick..The studies have been monitored by SEM, TEM, XRD and FTIR to corborate the results.

Bio-Diesel which is mono alkyl ester of vegetable oils, was produced from Oleaginous yeast *Trichosporon sps* yeast strain which has been isolated from decayed wood. Its potential to produce lipids has been evaluated on glucose, glycerol and sugarcane bagasse acid hydrolysate. The fermentation process was carried out for 120 h at 30 C. Lipids were extracted and subjected to transesterification using acidic Methanol (1% H_2SO_4). The mixture was heated at 60 C for 12h at alcohol/oil ratio of 6:1. and top phase containing fatty acid methyl esters (FAME) analysis of lipids was carried out by by GC-FID and NMR. It revealed the presence of Oleic acid, Palmitic acid, Linoleic acid and Stearic acid. The Biodiesel properties (Iodine Number, Cetane Number and cold filter plugging point) showed the sustainability of the yeast strain with potential for Biodiesel production. The cetane number of the lipids ranged from 53.39 to 59.59 indicating stability of Bio-diesel production. Sugarcane bagasse is one of the important lingo-cellulosic agricultural by-product which upon acid hydrolysis (1% H_2SO_4 with solid liquid ratio of 1:15 in autoclave for 30 mins) results in xylose rich stream. This can be utilized for the biosynthesis of lipids.. The possibility of using the biodiesel derived waste, glycerol and acid hydrolysate of agriculture waste for cultivation of yeast culture will simultaneously provide a method for the disposal of large volumes of algae biodiesel derived waste.

IT-02

Dust and NOx Reduction in Industrial Boilers by Iron-based Nanofluid

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A new Fe-nanofluid based heavy fuel oil additive, has been used for significant dust and NOx reduction in heavy fuel oil-fired smoke tube type boiler facilities successfully. The nanofluid contained particle size between 6 to 19 nm as confirmed by TEM analysis. The nanofluid was prepared from industrial waste containing iron sulphate. The method of preparation is simple and cost effective. NOx reduction was found to be 10.3% and 18.5% using additive active metal concentration of 1500 ppm in the boilers with steam generating capacities 0.2 tons/hour (fuel consumption 15 L/h) and 1.5 tons/hour (fuel consumption 150 L/h) respectively. NOx reduction was not influenced by the combustion hours. The furnace volume is smaller in small furnace and the flame fills up the whole furnace. Therefore, there is almost no temperature drop inside the furnace. At high temperature, more NOx is produced due to which Nox reduction is not apparent as it is compensated by more NOx formation at higher temperatures. Furthermore, there is less reduction environment for NOx reduction reactions in small boilers. In big boiler, large furnace volume is available and the flame fills up only about 1/3rd of it. This causes the temperature drop from 1400°C to 800°C at rear part of furnace. It results in less production of NOx. In addition, more reduction environment is available for NOx reduction reactions in big boiler. This may be the reason for improved NOx reduction in big boiler in comparison to small boiler.

The additive was found to reduce dust by 78.6% at an optimum active metal concentration of 30 ppm. On increasing the metal concentration input, the dust reduction was adversely affected. In presence of 30 ppm Fe content, the fixed carbon, ash and sulphur content of the dust were found to reduce. The dust reduction was not dependent on the boiler capacity. The dust particle size was analysed by laser diffraction method and the average particle size noted was 20 nm. The size of dust particles did not depend upon the additive concentration employed. The probable mechanism and reactions involved for NOx and dust reduction shall be discussed.

IT-03

Study on Allelochemicals from Some Indigenous Medicinal Plants

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The therapeutic properties of herbs had been recognized since creation of the universe. India is one of the oldest and richest floristic regions of the world and is well known for its ancient heritage regarding medicinal plants and plant drugs. All the major systems of medicine e.g. Ayurvedic, Unani and Homeopathy are largely based on drugs of plant origin. A large number of medicinal plants have been mentioned in Ayurvedic literature for their medicinal properties. Charak samhita and Sushruta samhita are good accounts for uses of plants in curing diseases of man and animals. 'Atharvaveda' contains 114 hymns or formulations for the treatment of diseases. Modern Allopathic system of medicine is also based on plants and herbs. Though a large number of synthetic drugs have been discovered and are used on large scale but the importance of plant based drugs can not be neglected because of their safety, efficacy, lower side effects and better compatibility with the human body. Thus research on plant products is playing a significant role in the drug delivery process of the pharmaceutical industry and various other research organizations.

The therapeutic importance of plants have been found to be attributed in several cases because of the presence of bioactive allelochemicals such as flavonoids, terpenoids, saponins, tannins, alkaloids and aromatic acids etc. Flavonoids especially their glycosides are the most abundant polyphenols. Recent studies have demonstrated that flavonoids found in fruits and vegetables may also act as antioxidants. In view of the significant importance of medicinal plants, isolation and characterization of allelochemicals from some medicinal plants and their biological importance are given in present lecture

Keywords: Allelochemicals, Plants, Biological Activities and Allelopathic Activity

IT-04

Friccohesity: New Physicochemical Standard to Engineer Surface Area and Activities of Thermodynamically and Kinetically Stable Nanoemulsions of Antioxidants

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Surface area and chemical activities are potential edges to harness the activities of industrial molecules on dispersing and solubilizing in suitable solvents. The molecular activities and surface area are directly related to a structure driven cohesive forces of medium vis-à-vis dispersing, binders and stabilizers. The cohesive forces or energy is weakened to disperse the ingredient or solute molecules in solvent. During dispersion the dispersing agent faces hindrances caused by the structure of molecules as they had cohesive forces. The hurdles in distribution are faced by the ingredient molecules vis-a-vis solvent cohesive forces due to structural networking of the solvent which opposes distribution. The opposing forces are noted as shear or the frictional forces. The stronger interactions of ingredients with medium develop stronger shear on the resultant liquid mixtures. The stronger cohesive forces favour more entangling of ingredients either in dispersion or the transportation. The stronger friction is attained by stronger weakening the cohesive forces and to create adhesive forces. A stoichiometric balance between cohesive and adhesive forces develops stable nanoformulations or nanoemulsion. The overall science and quality of nanoemulsion depend on the magnitude of cohesive and the friction forces. The kinetics of formulations is defined by a product of the cohesive and frictional forces and the product of cohesive and frictional forces is named as friccohesity. Therefore, weaker are the cohesive forces larger is the surface area and with a maximum surface area the formulations are noted as nanoemulsions. Nanoemulsion of antioxidants like flavonoids or curcumin expresses their substantial free radical scavenging due to their stronger surface activities. The cohesive forces, surface area, frictional forces, define distribution vis-a-vis activation energy, particle size, coagulability and coalescence, molecular or ionic hydrations. These properties are quantitatively determined with survismeter together saving 95% resources and human efforts. The survismeter is available in catalogue of Borosil Glass Works Ltd. In the lecture, the results of our studies will be discussed to signify the friccohesity as an authentic contribution for molecular interaction engineering of few antioxidants.

IT-05

Sustainable Development by Nano-Catalysis

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Although many organic reactions can be promoted by homogeneous or heterogeneous catalysis, but later offers many advantages such as easy workup, recyclability and less waste production.[1] The global concern about the climate change, energy production and conservation has prompted scientists to develop efficient recyclable heterogeneous catalysts for industrial processes. The study of heterogeneous catalysis has been a subject of intense study since the industrial revolution in the early 1800s.[2] Several solid base catalysts such as zeolites, metal oxides, mixed oxides, hydrotalcites etc. have been developed for the manufacture of organic intermediates and fine chemicals, among them metal oxides such as MgO, CuO and ZnO are of especial interest. During the synthesis of medicinally relevant molecules,[3] we became interested to develop nano catalytic system that can be used for more than one organic transformation. To achieve these objectives we synthesized various nano-materials and studied their catalytic potential for A3 and KA2 coupling and related organic reactions.[4] Some of the organic molecules synthesized during this work have been evaluated for antimalarial activity and have exhibited potent *in vitro* and *in vivo* antimalarial activity.

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IT-06

Graphene Oxide based Nanocomposites for Sustainable Catalysis

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The development of new smart materials is an evergreen areas of research for miscellaneous technological applications ranging from material science to energy storage and harvesting. These materials are the fulcrum of technological innovations of a nation. Today, the whole world is looking for development of smart materials for sustainable technologies.

Towards this objective, Graphene, after Carbon Nanotubes (CNT's), has become a new super star in the Carbon world and contributed immensely to the development of new smart materials.[1] Graphene oxide (GO) is the oxidized form of Graphene and it is one of the most versatile derivatives known. By virtue of its remarkable structural and physicochemical properties, GO alone or its composites have recently been used as heterogeneous catalysts in several organic reactions, thus making a significant contribution towards sustainable catalysis.

During the presentation, the synthesis and characterization of GO and its several composites i.e. GO-TiO_2, Go-MnO_2, GO-Cu, GO-Fe(0) will be discussed. The results of characterization of these new composites by FT-IR, FT-Raman, XRD, UV, TEM, FE-SEM, EDAX, TGA, N_2 adsorption–desorption and AAS analysis will be discussed. The catalytic potential of these new sustainable catalysts will be elaborated in the synthesis of amides, azo-derivatives, heterocyclic compounds and in the -C-H activation reactions.[2] Glimpses of our recent work on development of earth abundant metal composites of GO and their applications in sustainable organic catalysis will be presented.

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IT-07

Theoretical Chemistry as a tool for Designing Novel Organic & Inorganic Compounds for Synthetic and Biological Applications

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Theoretical chemistry is the platform for green synthesis of compounds having synthetic and biological applications. Different methods/packages have been introduced by chemists as well as physicists which are useful to predict the properties of potential organic & inorganic compounds to be used in synthetic and biological fields. Applications of DFT methodologies to predict properties like electrostatic potential surfaces, geometrical observations, spectral studies (FT-IR, UV-Vis, Raman, NMR), HOMO–LUMO, NBO and spin-allowed singlet-singlet electronic transitions studies (TD-DFT) by the B3LYP/6-311++G(d,p)/ LanL2DZ basis set levels of theory for calculating different properties by DFT methods to show reliability of theoretical data. VEDA 4 (Vibrational energy distribution analysis) software was employed for theoretical FT-IR spectrum analysis for fundamental vibrational modes along with potential energy distribution percentage (PED%) of compounds especially of Zn(II) complexes of dithiocarbazate Schiff base compounds. Thermal analysis data of the Zn(II) complexes up to 800 ^{0}C will be discussed, in addition to this bio-efficacy of the compounds have been examined against the growth of bacterial strains namely gram-positive *S. aureus* and gram-negative *E. coli* to evaluate their anti-microbial potential.

IT-08

Environmental Concerns of Tourism in North Western Himalayas

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The Himalayan region is endowed with huge tourism resources; yet its development has lead to serious environmental consequences. The special characteristics of mountains also called ‘mountain specificities’ are commonly considered developmental constraints. These specificities include inaccessibility, fragility, vulnerability and diversity (Berks & Gardner, 1997). Every developmental activity leads to environmental change (positive or negative). Tourism has the potential to contribute in a positive manner to the development of local communities but at the same time its uncontrolled growth can be the major cause of environmental degradation. Kashmir valley is one of the leading sought after tourist destination in the north western Himalayan region. However the

absence of a sound tourism policy coupled with phenomenon of mass tourism in the selected tourist destinations have trigged serious environmental and ecological concerns. The focus of the present paper is to evaluate the environmental status of one of the leading tourist destinations of Kashmir valley namely, Sonmarg by analysing the impact of tourism on land use/ land cover, water quality and solid waste generation.

Keywords: Sonmarg, Land use, Degredation, Destination

IT-09

Spinel-Type Cobalt Oxides: An Efficient Electrocatalyst for Electro-oxidation of Alcohol in Alkaline Medium

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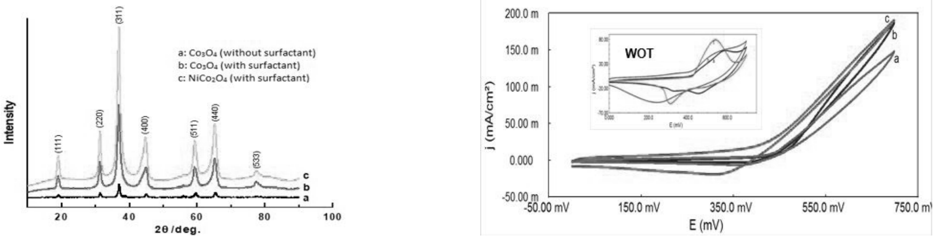
Spinel-type oxides of Ni and Co have been prepared at low temperature by using egg-white sol-gel route. Some analytical techniques such as, X-ray diffraction (XRD), FESEM/EDS and FTIR are used to characterise the material physicochemically. These investigations indicated the formation of almost pure spinel-oxide with micro-porous appearance. The electro-oxidation of alcohol has been performed in a three-electrode single compartment glass cell using an electrochemical work station (GAMRY Reference 600) provided with potentio-galvanostat and software installed personal computer. Electrochemical techniques like cyclic voltammetry (CV) and anodic polarization were adopted to study the oxidation process. Pt-foil, oxide film electrode and Hg/HgO/1M KOH were taken as counter electrode, working electrode and reference electrode, respectively. The oxide film electrode was prepared by suitable method on Ni or Pt support. Electrical contact of the oxide film was made with copper wire using silver paint and Araldite.

The anodic polarization curve of each oxide electrode was recorded in 1M KOH solution at 25°C with and without methanol. The study indicates that the oxidation process initiated relatively lower potential in the presence of methanol. The order of reaction was determined both with respect to [OH^-] and [CH_3OH] and found to be approximately unity in each case. Thermodynamic parameters ($\Delta H_{el}°^{\#}$, $\Delta S°^{\#}$ and $H°^{\#}$) were estimated from the Arrhenius plot obtained by recording the polarization curve in the presence of methanol at different temperatures. In the cyclic voltammetry study, no any redox peak was observed with the presence of methanol. This also authenticated the initiation of oxidation process at lower potential. The investigation may further be extended to fuel cell applications.



a: Co_3O_4 (without surfactant); b: Co_3O_4 (with surfactant) c: $NiCo_2O_4$ (with surfactant)

WOT: without methanol; WT: with methanol

IT-10

MOF in Green Chemistry

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ABSTRACT

Remarkable progress is going on mesoporous metal–organic frame works (MOFs)/ porous coordination polymers (PCPs)/ Porous materials, exhibiting exceptionally high surface areas and tunable pore features, excellent chemical stability and flexible surface structural functionality. MOF materials are composed of metal ions (or clusters) and coordinating linkers which impart high porosity to the MOF structures. Their extraordinary porosity and functionality from metals and organic linkers make them one of the most promising materials for a vast array of applications. The easy tunability of their pore size and shape from the micro-to meso-scale, by changing the connectivity of the inorganic moiety and the nature of the organic linkers, makes these materials special. Moreover, by combining with other suitable materials, the properties of MOFs can be improved further for enhanced functionality/ stability, ease of preparation and selectivity of operation. Curcumin consists of highly conjugated 1, 3-diketone moiety which can exist in several tautomeric forms, including a 1,3-diketo form and two equivalent enol forms. Curcumin shows anticancer potential in addition to its anti-oxidative, anti-inflammatory, anti-HIV and anti-angiogenic therapeutic properties. Curcumin having linear, planar and rigid structure is likely to benefit the formation of porous and stable frameworks. Therefore MOF has been synthesized using zinc acetate dihydrate and mixed solvent of DMSO and absolute ethanol. The structure has been well characterized by single crystal X-ray as well as other spectroscopic techniques results are correlated with the photoluminescence (PL) spectroscopy studies. The formed MOFs likely to provide source of less toxic Zn(II) as the metal source and an active pharmaceutical ingredient curcumin.

Keywords: Metal–organic Frameworks, Metal ions, Organic Linkers, Porous Materials

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IT-11

Latest Development for Food Industry Waste Management

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The Indian food retail market is expected to reach Rs. 61 lakh crore (US$ 915 billion) by 2020. The Indian food processing industry accounts for 32 per cent of the country's total food market, one of the largest industries in India and is ranked fifth in terms of production, consumption, export and expected growth. Food industry produces large volumes of wastes, both solids and liquid, resulting from the production, preparation and consumption of food. These wastes pose increasing disposal and can pose severe pollution problems and represent a loss of valuable biomass and nutrients. Large quantities of both liquid and solid wastes are produced annually by the food processing industry. These waste materials contain principally biodegradable organic matter and disposal of them creates serious environmental problems. Factors affecting the costs of waste disposal are the volume or hydraulic load and the strength or organic load. The waste loads at the processing plant can be reduced significantly through the use of new or modified processing methods and through in-plant treatment and re-use. A number of waste treatment processes are available to make the wastewater suitable for discharge. The most widely applied processes are biological treatment, impounding in storage lagoons and land irrigation. Most solid wastes are disposed of by returning them to the land. The key to minimizing the disposal cost is to remove excessive moisture from the wastes. Many opportunities exist for better utilization of food processing wastes. A variety of processes have been developed for converting the waste materials into bio-fuels, food ingredients and other valuable bio-products.

IT-12

Food as Medicine

R.S. Kaler

Let food be your medicine and medicine be your food. In order to combat the diseases (namely heart disease, cancer and injuries), we need to target individuals' poor health choices and habits and develop appropriate tools for population communication which can effectively change behavior. Antioxidants, phytochemicals, phenolic compounds, flavanoids, vitamins, minerals, proteins, enzymes and many more are natural substances in foods. They protect from disease by preventing the harmful effects of oxygen free radicals on your body. Oxygen free radicals are formed as cells in your body combine with oxygen to make energy. Free radicals also come from smoking or being exposed to radiation or sunlight from the environment. Herbs like Ginseng (may slow aging process by improving body's ability to use and absorb oxygen), Ginkgo Biloba (enhances age-related memory impairment), Green Tea (benefits immune system, protection from cancer and strokes, lowers blood pressure), **If we choose to live healthfully beginning, it can not only add years to our life, but life to your years.**

IT-13

Analytical Studies on Life Drugs and their Pharmaceutical Preparations

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The present research paper deals with the milligram determination of some Antibiotic drugs: Amoxicillin, Ampicillin, Cefixime, Cloxacillin Sodium, Norfloxacin and Ornidazole (pure samples) and their pharmaceutical preparations with Ammonium hexanitratocerete (IV) reagent in nitric acid medium.

An aliquots containing 1-5 mg of the sample were taken in 100ml stoppered conical flask followed by addition of 5ml AHC (0.1M) reagent, prepared in 0.5N-HNO_3. The reaction mixture shaken well and allowed to react for required time of room temperature (25-30^{O}) after the reaction was over unconsumed Ce(IV) was titrated against 0.025M FAS using ferroin as indicator. A blank experiment was also run under identical condition using all the reagent except the sample. The recovery of the sample was calculated with the amount of AHC consumed for the sample.

For every sample percentage error, S.D & C.V calculated, the method in simple, quick, convenient and accurate and perform in an ordinary laboratory condition without using any sophisticated instruments. The precision & accuracy was $\pm$ 1%.

Keywords: Analysis, Antibiotic, A.H.C., Pharmaceutical Preparations

IT-14

Synergistic Effect of Cl- on the Corrosion Inhibition of Mild Steel in 0.5 M Sulphuric Acid by Gelatin as a Green Inhibitor: Kinetics and Thermodynamic Studies

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Gelatin as a green corrosion inhibitor and it's adsorption properties with Cl- for the corrosion inhibition of mild steel in 0.5M sulphuric acid were studied using potentiondynamic,gasometric, weight loss and thermometric monitoring corrosion. The results shows that Gelatin inhibited the process of corrosion of mild steel. Gelatin was found to function by being adsorbed on the surface of mild steel. Gelatin shows synergism with Cl- and inhibition increases with concentration of Cl-. The adsorption of the Gelatin followed Langmuir adsorption isotherm. and Kinetic and thermodynamic parameter also measured and discussed.

Keywords: Mild Steel, Adsorption, Corrosion Inhibition, Gelatin, Synergism

IT-15

UV Curing Technology: A Greener Route for Fast Photocurable Acrylic Systems

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UV curing is an environmentally clean and efficient technique for radical initiated fast photopolymerizable systems. No solvents are used and the formulations are 100% solid systems leaving no volatile toxic residues.

It has a number of advantages over conventional curing systems due to ultra fast polymerization rates, low volatile organic emissions and room temperature operations with low energy consumptions. These light mediated reactions are very fast and take a few seconds to cure the system completely and thus greatly enhance the production rate. Differential photocalorimeter is an effective tool to investigate the photocuring behaviour and thermal properties of the cured polymers. The photocurable compositions may find suitable applications in lamination of transparent laminates, adhesives, UV coatings etc.

IT-16

Quantification of Hydrogen Bond Strength based on Interaction Coordinate: A New Approach

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Recently, we have proposed a new tool as 'Aromaticity Index Based on Interaction Coordinates (AIBIC)'[1] for the quantification of aromaticity which outcomes were satisfactory and encouraging. Encouraged by the recent served technique, a new approach to quantify the hydrogen bond strengths based on interaction coordinates (HBSBIC)[2] is proposed and is very promising. In this research, it is assumed that the projected force field of the fictitious three atoms fragment (D-H---A) where D is the proton donor and A is the proton acceptor from the full molecular force field of the H-bonded complex characterizes the hydrogen bond. The "interaction coordinate (IC)" derived from the internal compliance matrix elements of this three-atom fragment measures how the D-H covalent bond (its electron density) responds to constrained optimization when the H---A hydrogen bond is stretched by a known amount (its electron density is perturbed by a specified amount). This response of the D-H bond, based on how the IC depends on the electron density along the H---A bond, is a measure of the hydrogen bond strength. The inter- and intramolecular hydrogen bond strengths for a variety of chemical and biological systems are reported.[3] When defined and evaluated using the IC approach, the HBSBIC index leads to satisfactory results. Because this involves only a three-atom fragment for each hydrogen bond, the approach should open up new directions in the study of "appropriate small fragments" in large biomolecules.

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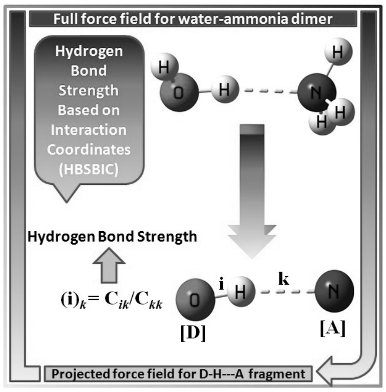

Schematic Diagram of the Presenting Work

IT-17

Synthesis, Characterization and Antimicrobial Ativities of Some Novel 2-Azetidinones Derived from Cyanoethyl Tertiaryamino Benzaldehydes

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Present report is the synthesis, spectral characterization and *in-vitro* antimicrobial activity evaluation of a series of azomethines and 2-azetidinones. Cyanoethylated tertiaryaminobezaldehydes were prepared by cyanoethylation of the corresponding aromatic primary amines followed by formylation in presence of $POCl_3$ and DMF. Cyanoethylated tertiaryaminobenzaldehydes on condensation with different aromatic primary amines afforded azomethines, which on cyclization with chloroacetylchloride and triethylamines in 1,4-dioxan gave new 2-azetidinones. All compounds were prepared by reported methodology and characterized by elemental analysis, FT-IR and ^{1}HNMR data. Further screened *in-vitro* for antimicrobial activity against *S. aureus, B. subtilis*, *P. vulgaris, E. coli, A. niger* and *A. fumigatus*. Most of the compounds showed activity against tested strains. The work shows the emergence of a new series of compounds in the field of antimicrobials.

IT-18

Transition Metal Nanocrystalline Spinel Ferrites: Green and An Efficient Heterogeneous Catalyst for one-pot Multicomponent Reactions

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The applications of transition metal nanocrystalline spinel ferrite as catalyst in organic synthesis performed through multicomponent reactions is an attractive area of research and most important processes for the preparation of highly functionalized organic compounds. Transition metal nanoferrites catalyst addresses the sustainability concerns and provides alternative efficient methods for various important organic transformations in the field of heterogeneous catalyst. In the present work, we have prepared transition metal nanocrystalline soft ferrites [MFe_2O_4, M (II) = Mg, Cu, Co, Ni and Zn] prepared by co-precipitation method and hard hexaferrite

using solution combustion method. The synthesized materials were characterized by thermal analysis, powders X-Ray diffraction, SEM and FTIR analysis for evaluating phase, structure and morphology and stoichiometry. X-ray diffraction confirms the formation of single phase nanocrystalline spinel ferrites with average grain diameter ranging between 25.00 to 30 nm. In order to know the magnetic hysteresis interactions, the magnetic measurements were carried out at room temperature by using SQUID Magnetometer with a maximum applied field of ± 5 T. The catalytic performance of nanocrystalline spinel ferrite towards the synthesis of 2-3 dihydroquanozolin 4(1H) one, 3, 4-dihydropyrimidin-2(1H)-ones/ thiones, Hantzch 1,4-dihydropyridine, tetrahydrodipyrazolopyridine and benzoxazin-ones/thiones derivatives with varied substitutions have been undertaken. The effects of solvents, amount of catalysts, reaction temperature and time of conversion etc. were also studied. This protocol offers several advantages including its greenness with respect to mild reaction conditions, good yields, short reaction time and operational simplicity. The catalysts retain their activity and product yield up to four cycles. The formation of compounds were confirmed by using FT-IR, ^{1}H & ^{13}C NMR spectral analyses and data compared with reported values.

IT-19

Toxic Chemicals all Around us: Is Green Chemistry the Answer?

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We strive to develop new technologies and processes yet often fail to consider their impact on environment and health. Green Chemistry provides one such alternative to prevent further environmental damage and promotes sustainability through the development of eco-friendly products.

Green Chemistry Network Centre (GCNC), established under the American Chemical Society's IUPAC CHEMRAWN GCI-DEN Grant and recommendation of World Leaders in Green Chemistry headed by Professor Paul Anastas (known as father of Green Chemistry), is working very hard to popularize Green Chemistry in India. The Centre provides a network for exchange of expertise, discussion and knowledge between industrialists and academicians and between chemists and engineers with interests and expertise relevant to Green Chemistry. The presentation will talk about new developments that have taken place to inculcate the significance of Green Chemistry. The presentation will also demonstrate some green chemistry experiments taken from a monograph published by us along with a real-world case of Indian Pharmaceutical Industry. Besides these, the Centre is also working on sustainable and socio-economic solutions for the problems associated with classical and emerging metal contaminants in water. Our group has also designed and synthesized new magnetically retrievable silica based organic-inorganic hybrid nanocatalysts and efficiently applied in various organic transformations. This work was published in RSC Green Chemistry Journal and it was most downloaded article. Moreover, recently we have edited a book for RSC Green Chemistry Series entitled, "Hazardous reagent substitution" that offers an extremely useful guide to arrive at safer reagents for synthesis of not only pharmaceutically relevant molecules but also for useful materials deployed in diverse domains. With these valuable benefits, green chemistry opens a field for innovation and new ideas for the future chemists to develop clean products and technologies.

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IT-20

Green Chemistry in Pharmaceutical Industry: A Case Study of an Antibiotic

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Green chemistry pledges to transform the chemical industry cleaner, safer and purer. The principle of such chemistry is based on the novel approach- benign by design- that supports the dual impact on human beings and on the environment. Supercritical fluids can be replaced conventional toxic solvents since many chemical processes need high temperature, volatile & toxic solvents and other volatile toxic compounds (VOCs). Solvent residues in the drug after manufacture might be fatal and/ or toxic to the treating patient and to the environment. Degradants of the drug may face similar consequences. Pharmaceutical and biotechnological industries are emerging as most active industrial sectors in the near future due to rapid expansion of genomics and to treat the undetected and unusual diseases. The presence of pharmaceuticals, degradants and other organic pollutants have been confirmed recently in the US, Japan, Germany, Hongkong, Taiwan, Vietnam and many other countries. Drugs can be degraded naturally through hydrolysis, biodegradation, direct or indirect photolysis and other means. Ubiquitous identification of a large number of drugs such as antibiotics, hormones, non-steroidal anti-inflammatory drugs (NSAIDs), β-blockers, psychiatric drug, lipid regulators etc. in reservoirs, lakes and rivers around the globe have been reported. Waste streams from pharmaceutical industry, hospital, waste water and sewage treatment plants have been earmarked as principal contributors to environmental pollution with human-derived medications. Green solvents, less toxic chemicals and safer ingredients should be preferably considered in order to make the earth ecofriendly. To make the environment, especially air-water-soil, greener and safer, it is essential to identify biologically and pharmacologically relevant characteristics of the chemical compound that are predictable and computable from the structures by the advanced quantum chemical study. The physicochemical, topological and electronic properties are to be ascertained, determined and analyzed in due manner. In an effort to do so, a first generation semi-synthetic antibiotic has been chosen as a case study. Cephradine (CEP) is orally administered having a broad spectrum of activity against gram positive and gram negative bacteria along with multiple applications. CEP has two nucleophilic sites and two hydrolysable groups with two ionized states. A Quantum Chemical Computational study on CEP and its degradants has been carried out with Gaussian 16 and Hyperchem 8 software packages. The thermodynamic properties both in vacuo and aqueous media have been compared to identify the potential and favourable hydrolysis pathways. Spectral and temperature dependent Monte Carlo Simulation data are of supportive to the experimental data. The carboxyl group attached with the said drug tends to act as a vital role in the hydrolysis pathways of such kind of antibiotics. Molecular docking of CEP with the target human prostaglandin synthase protein (1PYY) was conducted to visualize and interpret the hydrogen bond interactions and hydrophobic interactions of the best poses of drugs using Autodock Vina and Accelrys Discovery Studio. This sort of detail quantum chemical study is proved to be a viable and effective tool for novel drug design and synthesis in transforming the pharmaceutical industry safer and greener.

IT-21

Environmental Pollution Due to Recalcitrant Organic Compounds of Pulp Paper mill Waste Water After Secondary Treatment and their Challenges for Detoxification

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Pulp paper wastewater is major source of environmental pollution due to discharge of huge amount of recalcitrant residual organic pollutants even after secondary treatment. There is generation of 190-200m^3 of wastewater per ton of paper production. In India there is about more than 600 pulp paper industries which reflect the magnitude of the problem. The major identified compounds are: *1-(2,5-dimethoxyphenyl)-propanol, 9,12-octadecadienoic acid(z,z)-2,3-dihydroxypropyl ester, Octadecenoic acid, trimethylsilyl ester, Pentadecanoic acid, ethyl ester, (5α)-cholest-7-ene, β-Sitosterol trimethylsilyl ether, Silane, trimethyl[[(3β,5α)-stigmastan-3-yl]oxy]-, Pentane, 2-methyl-4-keto-2-trimethylsiloxy, 2-methoxy phenol, Phenol,4-ethyl-2-methoxy, 1-Tetradecene, Ethyl-2-octynoate, Tetradecanoic acid methyl ester, Hexadecanoic acid, cis-9-Hexadecenoic acid, trimethylsilyl ester, Hexadecanoic acid, trimethylsilyl ester or Palmitic acid TMS, Octadecenoic acid, trimethylsilyl ester, Octacosane, Silane, [[(3β)-cholest-5-en-3-yl]oxy]trimethyl-, β-Sitosterol trimethylsilyl ether*; which has been reported not only as toxic due to contribution of pollution parameters i.e. BOD, COD, heavy metals etc. but as mutagenic and carcinogenic also. Therefore, the detoxification of these compounds is essential prior to its discharge into the environment. The biostimulation and biodegradation has been found as effective technology for the detoxification of discharged effluent at tertiary stage treatment by providing the adequate source of nitrogen, carbon and oxygen. The identified potential autochthonous bacteria i.e.: *Klebsiella pneumoniae* IITRCP04 (KU715839), *Enterobacter cloacae* strain IITRCP11 (KU715840), *Enterobacter cloacae* IITRCP14 (KU715841) and *Acinetobacter pittii* strain IITRCP19 (KU715842) were found capable for degradation of various recalcitrant organic compounds during biostimulation process. The use of biostimulation and bioaugmentation process may be an effective detoxification technology for pulp paper mill wastewater. Further, the detoxified wastewater can be re-used for sustainable development. Hence, the developed novel technology may be as boon for prevention of river pollution and conservation of aquatic resources.

IT-22

Synthesis of Nanostructured Metal Oxides in Polymer Matrix for NO_2 Gas Sensing Applications

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My presentation will include the research work carried out on various nanostructured metal oxides such as ZnO, SnO_2, TiO_2 etc. and their composites with polymeric materials like PANI, PEG, PVA, polypyrrole etc. As special case I will discuss the preparation of ZnO thin film, polyaniline (PANI) and PANI-ZnO and their applications as NO_2 gas sensor. Pt-doped SnO_2 thin film based sensor was found to give maximum sensing response of about 183 towards low concentration of (20 ppm) of NO_2 gas at the temperature of 90°C with very fast response (~ 6 sec) and recovery (~ 13 sec) time. Amongst all the prepared sensor structures, the SnO_2-ZnO (ZSO) sensor structure showed a high sensing response of about 1578 towards 20 ppm of NO_2 gas at a lower operating temperature of 70°C with an average response and recovery time of 3.91 min. and 6.91 min. respectively. These results as the film properties and sensing performances have been discussed in terms of a space-charge layer formed on the columnar grains.

Keywords: Nanostructured Metal Oxide, NO_2 Sensor, Thin Film

IT-23

Impact of Environmental Cadmium Pollution on Metabolic Modulations and Antioxidant Enzymes in Heart and Muscle of Rabbit

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Cadmium is a naturally occurring minor element, one of the metallic components in the earth's crust, oceans and present profoundly in our environment. Cadmium (Cd^{2+}) is one of the most common nonessential elements, relatively accessible heavy metal in our environment causing wide range of toxic effects. Since 1930s, worldwide awareness for cadmium was increased steadily to the extent that its consumption now limited to essentially by the concentration of cadmium in zinc ores and the supply of refined zinc (Lymburner, 1974; Hiatt *et al.*, 1975).

A person's daily intake may be as little as 0.05 milligrams and is stored in the whole body in an average of 50 milligrams. Cadmium levels are estimated to be between 0.1 and 0.2 ppm within the earth's crust, making it the 67th element in order of abundance. The average level of cadmium in unpolluted soil is about 250 ppm. It is therefore naturally present predominantly in air, water, soils and foodstuffs. With the discovery of new uses of cadmium, the problem of its adverse effects also intensified. Because of its potential for uncontrolled widespread introduction into the environment, cadmium is designated as "The dissipated element". Small industrial domestic use of cadmium products will emit low levels of cadmium to the environment.

Blood cadmium concentrations were mainly associated with tobacco smoking (partial r2 = 0.56; $p < 0.0001$), while consumption of caribou liver and kidney remain a minor source of cadmium exposure among never smokers. Cadmium has been found in at least 776 of the 1,467 National priorities List sites identified by the Environmental protection Agency (EPA). The incidence of cardiovascular disease has increased in the general population and cardiac damage is indicated as one important cause of mortality. Although recent investigation have established that free radicals may be important contributors to cardiac dysfunction and myocardial damage. Impact of Cd in drinking water on plasma lipoprotein and blood pressure has been studied in male white pigeons by Revis *et al.,* (1988) and reported that a significant decrease in LDL protein, LDL cholesterol and a significant increase in systolic, diastolic blood pressure and aortic plaque size, which clearly revealed the cardiovascular effects of cadmium.

In our laboratory Mohana Radhika [2008] reported that the cadmium toxicity could have induced oxidative damage in both liver and kidney by enhancing peroxidation of membrane lipids due to inhibition of the antioxidant enzymes. Subba Rao [2010] has been carried some investigations in our laboratory and reported cadmium toxicity induced alterations in heart and muscle tissues of rabbit leading to changes in blood constituents, abnormalities in heart and muscle function altering glycolysis, citric acid cycle, phosphotase metabolism, transamination reactions and induction of free radical stress.

IT-24

Semiconductor Nanostructured Based Sensors for Monitoring Air Pollution

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Detection of minor gas leaks in a hazardous work environment has been a challenging research problem for many decades as it involves health, safety and environmental risks. The past decade has shown enormous research contribution in terms of publication to achieve high quality sensor. A recent report of the World Health Organisation has revealed Gwalior is the most polluted city in India in terms of air pollution along with other 12 cities of India. The report also suggests that the Indian population living outside Kashmir and the Himalayan belt are exposed to air pollution beyond the WHO safe limits. Meanwhile, Delhi, touted as the most polluted city in the world, doesn't feature in the list of cities with highest air pollution levels. Also, no other metro city features in the notorious list. Both experimentalists as well as theoreticians have tried their level best to design

and miniaturize sensor materials. Some of them got well recognition but still the goal to achieve quality sensor is far apart. Conventional sensors based on semiconducting metal oxide thin films, organic polymeric materials, silicon and carbon black-polymer composites have been preceded by nanostructure sensor for past decade. In this race, carbon nanostructures evolve as prominent candidate because of its extraordinary chemical and physical properties. 1D and 2D-nanostructures served fascinating research prospects for scientific community in past few decades. Starting with carbon nanotube (CNT) and graphene different new 1D and 2D nanostructures have been introduced with novel chemical and physical characteristic. These nanostructures are expected as quality sensor materials and are essential for miniaturizing electronic devices. The present talk will include our group's recent computational work on 1D and 2D nanostructures for their sensor application for Air and Water pollution, using density functional theory approach. Analysis has been made in terms of bandstructure, density of state, charge transfer and current voltage (I-V) characteristic.

IT-25

A Thermodynamic and Comparative Study of Pharmacetical Drug (Paracetamol) by Ir(III) and Pd(II) Catalysed Oxidation in Acidic Medium($HClO_4$): Kinetic Model

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A comparative study of Pharmacetical drug (Paracetamol) by Ir(III) and Pd(II) catalysed oxidation in acidic medium ($HClO_4$] at 35 ^{0}C to 45 ^{0}C. The reaction is carried out in the presence of mercuric acetate as a scavenger for bromide ion. 1-carboxy cyclohexane l-acetic acid was obtained as the oxidation product and identified chromatographically. The rate law followed a first order and zero order dependence with respect to $KBrO_3$ and potassium chloride [KCl] respectively. The reaction followed first order with respect to Ir(III) and Pd(II) chloride. Negligible effect of [$Hg(OAc)_2$] and ionic strength of the medium was observed. The rate of reaction decreased with increasing [H^+] was observed for the oxidation of paracetamol. Rate of reaction exhibits fractional positive order kinetics with respect to [PA]. The values of rate constants observed at different temperatures (30 to 45^{0}C) were utilized to calculate the activation parameters. Quinoneoxime and acetic acid have been identified as main oxidation products of the reactions. Feasible mechanism is proposed which are be composed with the kinetics, stochiometry and product of the reaction. The rate law has been derived from obtained kinetic data.

Key Words: Kinetics, Ir(III) Chloride, Pd(II) Chloride Oxidation, Paracetamol, Potassium Bromate, Acidic Medium.

IT-26

Global Warming and Climate Change Issues: Challeges and Slutions

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Global warming of planet earth and climate change issues has become the foremost challenges endangering the sustainability of life on the earth. Natural i.e., geological activities and anthropogenic emissions mainly the greenhouse gases like laughing gas (N_2O), plants food (CO_2), marsh gas (CH_4), Freon (CFC) and Ozone (O_3) with its paradoxical behavior etc. have been interrogated as the chief contributors to the phenomenon and to curtail their emission is a great challenge before modern society. Global warming and climate change severely affecting the behavior and pattern of Indian monsoon causing threats of flood and drought with many other adverse impacts to the environment. It is amendable to curtail and control air pollutants chiefly the greenhouse gases from the cities worldwide. With global support and vision a global/ local/ regional action plan and a better understanding of the interrelationship among the greenhouse gases, warming and climate change is needed to combat the problem effectively. The present study aims at the review of the warming and climate change issues in both local and global prospective. To mitigate the warming issues green building concept in smart cities are being taken into account. This review paper will may help to make awareness development and more focused research and development planning which primarily needed this time.

Keywords: Global warming, Green building, Climate change, Pollution Climatology, Greenhouse Gases, Smart city

IT-27

Computer Aided Designing of New Compounds

(A Supportive Method to Wet Lab.—A Greener Approach)

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It is a demand of today's world that the chemical sciences should develop and design new and useful compounds for the service of mankind without using methods which are traditional one. Scientific workers were trying to develop and synthesizing series of new compounds since past in the wet laboratories using traditional synthetic methods and they used to check their properties thereafter. The process seems to be time consuming and which leads to synthesis of number of compounds. Some of the recent trends have been

emerged and developed in the field of designing of compounds with greener approach. These may include microwave synthesis, computer aided designing etc.. This presentation will focus on computer aided designing i.e. studying and designing of compounds on the PC first without trying a lot of synthesis in the wet lab.. These computational methods are less time consuming, involve less chances of error, and are helpful in control of pollution. These methods may also prove to be helpful in designing compounds with desired properties. The presentation includes introduction to the computational methods, a little theory behind these methods, their applications and use of software/ s particularly the use of software/s of semi-empirical methods in the study of properties of compounds viz. Geometric and structural properties of compounds, QSAR studies and simulation of spectra of compounds on the basis of work done by our research group in this related field.

ORAL PRESENTATION (OP)

OP-01

Synthesis of Zinc Metal MOFs: An Aqueous Phase Selective Sensors for Picric Acid

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Currently, the quick, reliable and precise detection of explosives has become a major concern in the perspectives of speedily growing explosives deployments. Metal Organic Frameworks (MOFs) are permanently porous crystalline coordination networks composed of two main components (organic linkers and metal centers). Metal organic frameworks (MOFs) have received great attention in recent years, due to their fascinating architectures and topologies as well as their increasing properties and potential applications such as functional materials, magnetism, luminescence, catalysis, gas separation, gas storage and drug delivery. The synthesis of MOFs can be influenced by many factors such as the nature of metal ions and organic ligands, solvent system, counterions as well as molecular interactions including hydrogen bonding and $\pi-\pi$ interactions that can be used to govern the process of self-assembly. The term metal-organic frameworks describes a class of materials in which organic polyfunctional ligands mostly like 1,4-benzenedicarboxylic acid and 1,3,5-benzene-tricarboxylic acids form coordination bonds with some specific transition metals to form extended polymeric structures. Numerous studies on properties and chemical structures of MOFs have been done. Metal organic frameworks (MOFs) of copper and zinc synthesized with 1,4-benzenedicarboxylic acid and N,N-dimethylformamide at room temperature. The MOFs were characterized by Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (PXRD) and Luminescence. The results obtained are presented. In the present study, MOFs have been synthesized from two different solvents with same procedure.

Keywords: Zinc Metal organic frameworks, FTIR, XRD

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OP-02

Clay Catalyzed Green Synthesis of Isatin based Bio-active Heterocyclic Derivatives

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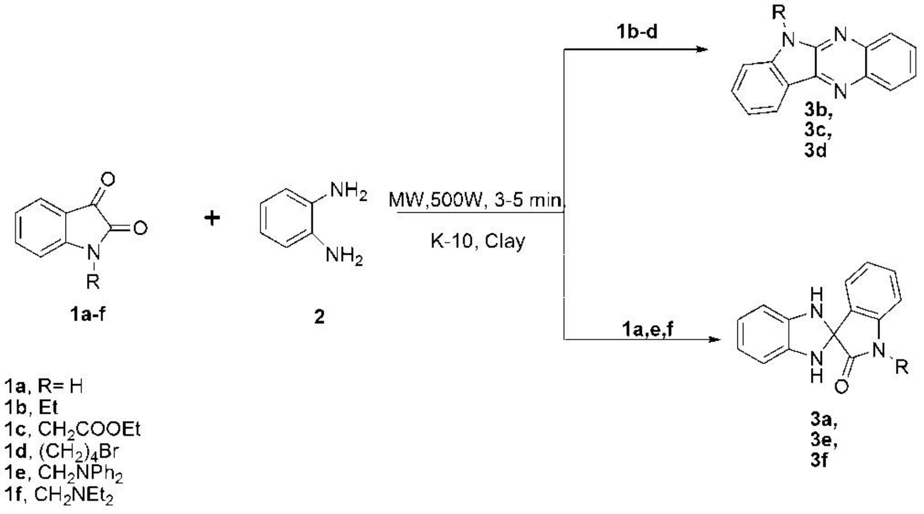
One of the major current challenges is to develop synthetic methods that are less polluting. In particular, the field of heterogeneous catalysis has captivated the interest of researchers due to an increasing demand for more environmentally acceptable processes in the chemical industry. In recent years, the use of solid acid catalyst such as clays, ion-exchange resins and zeolites has received considerable attention in different areas of organic synthesis. The chemistry of heterocyclic compounds has received considerable attention due to their synthetic and biological importance. Such compounds often exhibit potent antiviral and antibacterial properties. K-10 clay was identified as an efficient heterogeneous catalyst for the synthesis of various heterocyclic moieties. In the present method, some bio-active heterocyclic derivatives were synthesized by the reaction of isatin derivatives with o-phenylenediamine under microwave irradiation. The presented method is mild, environmentally friendly, inexpensive and highly effective to give the products in good to excellent yields. The recyclability of the catalyst is another emphasis of proposed methodology.



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OP-03

Comparative Study of Molecules Synthesized via Microwave and Classical Heating Techniques

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Synthesis of newer heterocyclic molecules has great importance for health sciences and chemical industries as well. With advancement of techniques and skills, microwave heating methodology has emerged as quicker, safer, greener and economical path way to synthesize chemicals over traditional heating. In the course of study preparation of different classes of compounds as quinoxalines, azides and azoles were studied. This paper reveals that these molecules yield better in microwave path way than via classical heating technique.

Keywords: Classical Heating Techniques, Microwave Heating, Greener, Quinoxaline, Azole

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OP-04

Terrestrial Carbon Sequestration in Different Land Use System in Dewa Block of District Barabanki, U.P. (India)

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Carbon is found in all living organisms and is the major building block for life on earth. In the environment, carbon exists in many forms—predominately as plant biomass, soil organic matter and geologic deposits and as the gas carbon dioxide (CO2) in the atmosphere and dissolved in sea water. Carbon sequestration is the long-term storage of carbon in oceans, soils, vegetation (especially forests), and geologic formations. Carbon sequestration is a needful method to develop a balanced ecosystem by controlling increasing GHG's. In agricultural systems, the amount and length of time carbon is stored in the soil is largely determined by how the soil resource is managed. The effects of land use change on soil carbon stocks are of concern in the context of international policy agendas on greenhouse gas emissions mitigation.

Present work emphasized on the influence of land use changes on soil C stocks and carbon sequestration potential in different land use system. Three different soil series of Dewa Block, *i.e.*, Gangauli soil series, Bajgahani soil series and Sihali soil series were selected for comparative study of soil carbon stocks and carbon sequestration potential in three different land use system *i.e.,* forested, cultivated and uncultivated lands. These soil series were categorized as per soil survey report of U.P Agriculture Department, Uttar Pradesh. The physical properties indicated that the Gangauli soil series was coarse loamy, very deep and well drained soil sand. Sihali Series was fine loamy, very deep, moderately well drained soils while Bajgahani Series was fine silt, very deep, poorly drained soils. Chemical properties indicated that surface soil pH were ranged from 6.85 – 7.66 in forested land, 7.73 – 8.5 in cultivated land and 7.62 – 8.76 in uncultivated land in different

soil series. The maximum soil pH was found in uncultivated land of Gangauli soil series (pH 8.76) and least pH in forested land of Sihali series (pH 6.83). Organic carbon content was also maximum in Forested area (0.88-0.95%). Medium in cultivated (0.5 – 0.705%) and least in uncultivated land (0.39% - 0.64%). Thus SOC stock was observed maximum in forested land (19.83 – 21.6 Mg/Ha), medium in cultivated land (11.68 – 20.79 Mg/Ha) and least in uncultivated land (9.3 – 16.23 Mg/Ha). Thus, result indicated that soil carbon sequestration potential in forested land was maximum (72.73 – 79.28 Mg CO_2/Ha), medium in cultivated land (42.83 – 76.25 Mg CO_2/Ha) and least in uncultivated (34.1 – 59.52 Mg CO_2/Ha). Thus it was concluded that land use system directly affect the soil carbon sequestration potential. So forested land use was maximum stored carbon in form of SOC and sequestration equivalent atmospheric carbon dioxide and least in uncultivated land.

OP-05

Enhancment of Carbon Sequestration Potential of Mulberry through Different Agronomical Practices

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The major issue of the twenty first century is to reduce the carbon foot print emerging at an alarming rate from energy, process industry, land-use conversion and soil cultivation. To address this problem, conference of the parties (COP21) initiative has been undertaken in order to increase the annual soil carbon stock by 0.4% and to halt the increase carbon dioxide content in the environment due to human activities. This can be achieved through sequestration of atmospheric CO_2 into other long-lived global pools including oceanic, pedologic, biotic and geological strata. Considering the large scale cultivation of mulberry in India, we hypothesized that it could capture the atmospheric CO_2 because of its higher biomass production capacity. Therefore, an attempt has been undertaken to enhance the efficiency of carbon sequestration potential of mulberry plant through different cultivation strategies. An experiment was conducted with six replications under split plot design, main plot as irrigation (furrow and drip irrigation) and sub plot as recommended package of practices with or without reduced tillage and mulching. Growth parameters and biomass yield of plants were recorded consequently for 3 years. The result indicated that maximum mulberry leaf yield was recorded in drip irrigation with reduced tillage and mulching (i.e. 13950 kg $ha^{-1}crop^{-1}$) than in drip irrigation without reduced tillage and mulching (13350 kg $ha^{-1}crop^{-1}$). The total amount of carbon sequestered by mulberry leaf as well as stem was higher in the former management practice (14,846 kg $ha^{-1}year^{-1}$) compared to later (14,204 kg $ha^{-1}year^{-1}$). Chemical analysis of soils among all the management practices indicated that drip irrigation with reduced tillage and mulching could maintain higher amount of high organic carbon content (8.5 g kg^{-1}), available phosphorus (72.23 kg ha^{-1}), potassium (407.88 kg ha^{-1}), copper (1.10 $\mu g\ g^{-1}$), zinc (3.30 $\mu g\ g^{-1}$), iron (3.25 $\mu g\ g^{-1}$) and manganese (1.30 $\mu g\ g^{-1}$) compared to others.

Keywords: COP21, Carbon Sequestration, Mulberry, Drip Irrigation, Reduced Tillage, Mulching And Available Nutrients

OP-06

Energy Efficient Buildings and Energy Saving

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A building which can run by best amount of energy, devour less water, preserve natural resources, produce less waste and produce spaces for healthy and comfortable living, as compared to conservative buildings, is a green building. Conservative methods of building exercise tremendous quantities of material, numerous of them non-renewable and toxic, and pay little attention to the impact the building has on the environment. Green buildings not only reduce these impacts but are also healthier and consume less energy saving money in the long run.

Green building design is a sensible and climate cognizant move toward building design. Various factors, like geographical location, current climatic conditions, use of locally available and low personified energy materials and design parameters relevant to the type of usage of the building are normally taken into consideration. Such an approach ensures minimum harm to the environment, while constructing and using the building.A green building uses bare minimum amount of energy, consumes less water, conserves natural resources, generates less waste and creates space for healthy and comfortable living.

When a number of green buildings are located in proximity, they would create a green zone, providing much healthier environment and minimise heat-island effect. The ultimate aim will then be to create many such areas, which would help the towns and cities and therefore the nation in reducing total energy requirement and also the overall global carbon footprint.

The building sector alone represents about 40% energy consumption. Actualizing the situation, the need of the day is to adopt sustainable green building design approach which is the ultimate solution to reduce the energy demand of the building.

OP-07

Lichens: Bio-tool to Predict the Green House Gas (GHG) Emissions

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Many chemical compounds present in the earth's atmosphere act as greenhouse gases. Some of these are natural in origin (water vapour, carbon dioxide, methane and nitrous oxide), while others are exclusively human-made (like gases used for aerosols). Levels of several important greenhouse gases have increased by about 25% since large-scale industrialization began around 150 years ago. The negative impact of rising levels of greenhouse gases is the global temperature rise resulting in rise in occurrence of extreme climatic events.

Although the complexity of the natural system sets fundamental limits to predictive modelling, the approach is useful in obtaining a first approximate estimate for the potentially dramatic impact of climate change on biodiversity. Thus, there is a need to find appropriate indicators to identify the effects of climate change, to verify results of modelling and to determine the response of species.

Lichens are considered as sensitive indicators of global warming, as the spread of several thermophilous epiphytes in north-western Central Europe has been attributed to late twentieth-century warming. In the recent years some thermophilous lichen species strongly increased in frequency mostly belonging to the physciaceae family. Studies have been carried out which revealed terricolous lichens respond to global warming as their distribution has been restricted due to warming phenomenon. In the Himalayas (Pindari region) green algae-containing lichens exhibit an increase in number than cyanolichen based on comparison of the past published account of lichens three decades earlier as well as there has been increase in trentepohiliod lichen species and decrease in soil- and rock-inhabiting lichens.

Biological monitoring with epilithic lichens involves lichen measurement along transects on flat calcareous rocks, and construction of a trend detection index (TDI) is a method based on total lichen species cover with coefficients chosen so as to ensure maximum ability to detect global climate trends.

In view of unique characteristics of lichens and their ability to withstand rising temperature, lichens are considered most appropriate indicators of GHG emission and to anticipate changes in the global climatic conditions.

OP-08

Impact of Climate Change on Biodiversity: Global Crisis

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Climate change is one of the most important global environmental changes, with implications for food production, water resources, health energy, biodiversity etc. The global temperature of earth may increase between 1.9 and 5.0 degrees Celsius by 2100. Biodiversity is the variety of different types of life found in earth and the variations with in species. This can refer to genetic variation, ecosystem variation with in an area, biome or planet. Biodiversity provides input for agriculture without which production would not occur. It contributes to climate stability, and maintenance of ecosystems. Impact of climate change on biodiversity is the more significant threat in the coming decades. Loss of Arctic Ocean ice, higher concentration of CO2 in the atmosphere is already being observed. In addition to warming temperatures, more frequent weather events and changing patterns of rainfall data on Himalayan glaciers indicates recession of some glaciers. CO2 in the atmosphere increases at the rate of 1.9 ppm per year. At present, the amount of CO2 in the atmosphere is 389 ppm as compared to oxygen which is 2,10000 ppm. Other gases contribute to warming are Chlorofluro Carbon (CFCs), methane, SO2, NO2 etc. Sea level rise is also the important impact of global warming because it affects coastal environments. At least since 1880, the average sea level has been rising. Changes in ocean temperature leads to threatening of marine life. Over the entire ecosystem will be affected and become imbalanced. The animals are also endangered due to climate change.

OP-09

Design for Environment and Waste Minimization: A Green Approach

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Design for the environment is a design approach to reduce the overall human health and environmental impact of a product, process or service, where impacts are considered across its life cycle. Design for Environment (DFE) is the original name of a United State Environmental Protection Agency (EPA) program, created in 1992, which works for the prevention of pollution and the risk of pollution for human being and environment. A environmental design process must be considered for conserving and reusing the earth's scare resources, where energy and material consumption is optimized, minimal waste is generated and output waste stream from any process can be used as the raw materials Different software tools have been developed to assist designers in finding optimized products and processes. Modern day businesses all aim to produce goods at a low cost while maintaining quality, staying competitive in the global marketplace, and meeting consumer preferences for more environment friendly products. To help businesses meet these challenges, EPA encourages businesses to incorporate environmental considerations into the design process. The benefits of incorporating Design for Environment include: cost savings, reduced business and environmental risks, expanded business and market opportunities, and to meet environmental regulations. Analysis tools can be used to identify broad environmental issues, but improvement techniques are needed in order to solve any problems identified. DFE strategies are sufficiently broad to be used at the product planning and problem definition stage of the design process.

Keywords: Waste Minimization, Cleaner Process, Zero Emission, LCA, Sustainable Development, Safer Choice

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OP-10

Synthesis, Spectroscopic and DFT Studies of tris(dimethylsilyl)methane $HC(SiMe_2H)_3$

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Tris(tridimethylsilyl)methane P_1, a bulky organosilyl precursor was synthesized by reacting chlorodimethylsilane with magnesium turnings and bromoform under inert conditions using double manifold vacuum line. The compound $HC(SiMe_2H)_3$ P_1 was then characterized by Mass, FT-IR, ^{1}HNMR,^{13}CNMR,^{29}SiNMR and UV- visible spectroscopic techniques.

Theoretical quantum chemical calculations were performed using DFT in combination with B3LYP exchange correlation functional and 6-311++G (d, p) basis set level. The computed parameters of the precursor P_1 were:

chemical potential (μ) -0.146905 eV, HOMO- LUMO energy gap- 0.26835 eV, chemical hardness (⍰) -0.13417 eV , softness (S) 2.094 eV, ionization energy (IE) -0.28108 eV , electron affinity (EA) -0.01273 eV, dipole moment (D) 0.7761 Debye, electronegativity (EN) 0.14690 eV, electrophilicity (W) 0.0801 eV and relative stabilization energy -1148.7307 eV. In the theoretical FT-IR spectrum analysis 90 fundamental vibrational modes has be observed because of non-linear structure of P_1. Theoretically calculated parameters like FT-IR, ^{1}HNMR, ^{13}C{^{1}H}NMR, ^{29}SiNMR and electrostatic potential and HOMO-LUMO energy gap are in good agreement with experimental results.

Keywords: DFT Studies, Bulky Silyl Group

OP-11

Waste Management through Engineering and Chemical Process for Alternate Energy Production and Reduce Pollution

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In India the number of vehicles on road is increasing with a very high rate. Presently, there are above 1.96 crore vehicles which is almost 53,720 vehicles hitting the road daily. These vehicles are the major source of replaced waste used tyre. It has become a severe problem to manage and deal with these waste tyres. At many places these tyres are simply buried in to the soil or openly fired which lead to soil as well as air pollution. On other side the fuel prices is also increasing with high rate. Hence, taking in to consideration the above point the present investigation was carried at G.B. Pant University for fuel production from these waste tyre. The conversion of waste tyre in to fuel is done by the pyrolysis processes. The obtained raw paralysed oil was further purified for its properties improvement by the chemical process of desulphurization and distillation. The obtained purified oil was further blended with diesel in different proportion for engine testing performance. It was observed that it is possible to produce oil from waste tyre through pyrolysis process. The obtained oil contained large amount of impurities which can be removed by the desulphurization and distillation process. The purified oil after blending with diesel up 40% can be used in the engine as substitute to diesel oil.

OP-12

Synthesis of Acridine Derivatives as an Anti-Malarial Agent

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N-[5-{(Acridin-9-yl)-2-chlorophenyl}alkyl]-aryl amides/imides was synthesized by taking the mixture of 4-chlorobenzoic acid (0.1 mol), diphenylamine (0.1 mol) and anhydrous $ZnCl_2$ (10g) and heated at 260°C

for 10 hrs, to get 9-(4-chloro-phenyl)-acridine crystals. A powdered mixture of 9-(4-chloro-phenyl)-acridine (0.05 mol) and an appropriate amido/ imido alkylol (0.05 mol) was dissolved in conc. H_2SO_4 to get target compound N-[5-{(Acridin-9-yl)-2-chlorophenyl}alkyl]-aryl amides/imides. Acridine derivatives as anti-malarial drugs were developed after the synthesis and evaluation of a large number of quinoline compounds. Among acridine derivatives that have been used clinically are acriquine, aminoacrichin, azacrin. The last compound was designed with a combination of 8-aminoquinoline and 4-aminoquinoline. Azacrin appears to be more effective schizonticide than quinacrine and acts more readily than chloroquine or amodiaquine in P. falciparum. A later development of a promising in acridine-10-oxide, which is more potant than quinacrine against P. lophure in ducks and P. knowlesi in monkeys. This compound has given promising result in clinical trials and does not produce yellow staining of the skin; its activity appears to be comparable to that of chloquine.

OP-13

Rapid Characterization of Secondary Structure by FTIR Spectroscopy in Bacidia Incongruens Commonly growing around Tanda and Unchahar Thermal Power Plants of Uttar Pradesh, India

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Fourier- Transform Infrared (FTIR) Spectroscopy was used to identify and determine the spectral features of secondary metabolites present in thalli of *B. incongruens*, a common lichen species found growing around two thermal power plants of the states of Uttar Pradesh. The plant material for the present study was procured from Tanda and Feroze Gandhi Unchahar thermal power plants and specific spectroscopic biomarkers for rapid identification and discrimination were analysed. FTIR analysis showed typical functional groups such as amino, carboxylic, phosphate and carbonyl on the surface of material studied that indicate the involvement of different functional groups in biosorption process.

Hence, the variation in the functional group bands in IR region shows the effect of pollutant on the functional group chemistry of the species. The wavelengths of prominent peaks obtained from the absorbance spectra showed the spectra of lichen species. It can be seen that, lichen species have good similarity in the spectra, in comparison between the obtained spectra of the lichen species; it is possible to point out on several spectral peaks.

FTIR spectra showed structural peculiarities of metabolites in lichens as well as variations in functional groups i.e. N-H stretching Amide-A, O-H stretching of hydroxyl groups and carboxylic acid (primary, secondary, amines and amides), SO_3 asymmetric, C-O bonding due to polysaccharides and C-Br stretching (alkyl halides) which indicates the role of metabolites in sequestration of metals through absorption phenomenon.

The spectra of *B. incongruens* around Tanda and Feroze Gandhi Unchahar National Thermal Power Plants showed presence of both primary and secondary metabolites which enhances the probability of detection of IR bands in 3500- 3300 cm^{-1}(showed the stretching of N-H/ O-H groups). The spectral band observed between 3000- 2800 cm^{-1} in all directions of the study area due to asymmetrical vibration of C-H showed the presence of protein and phospholipids. The range of wavelength 1560-1530 cm^{-1} showed the presence of C-N stretching, N- H bending with the presence of secondary amines. The range of wave number 1080-1010 cm^{-1} showed SO_3 asymmetric stretching and C-O bonding due to polysaccharides in all directions. The presence at absorbance band 770-620 cm^{-1} showed the presence of amines-V with out of plane NH bending. The peaks ranged between 690-515 cm^{-1} and 530-400 cm^{-1} resulted absorbance values in all directions of the study area due the vibration modes of C- Br stretching coupled to alkyl halides and the presence of vibrational frequencies of Al-O stretching (AlO_8 Octahedral; isolated) respectively. The useful ranges of metabolites provide data for rapid detection and characterization of lichen *B. incongruens* at different level around thermal power plant.

The observations are useful to detect rapidly and characterized the occurrence of lichen *B. incongruens* at different level of metal accumulation around thermal power plants. FTIR analysis provides spectroscopic evidence of the role of chemicals in metal absorption as the variation in the frequency is affected by bond dissociation and bond formation which plays important role in metal chelation. This study reveals vital information obtained by FTIR technique that can be used to understand the structure and stability of some peptides and proteins in different environments as well as wavelengths.

Keywords: Lichens, FTIR, Spectroscopy, Thermal Power Plants, Species

OP-14

Theoretical Insights into the Molecular Structure, Solvent Effect on Spectroscopic (IR, NMR and UV/Visible) Properties, Thermodynamic Properties, NBO, NLO and Biological Properties Evaluation of Novel 4-[Bis [2-(Acetyloxy) Ethyl] Amino] Benzaldehyde (BAEAB): A DFT and TD-DFT Approach

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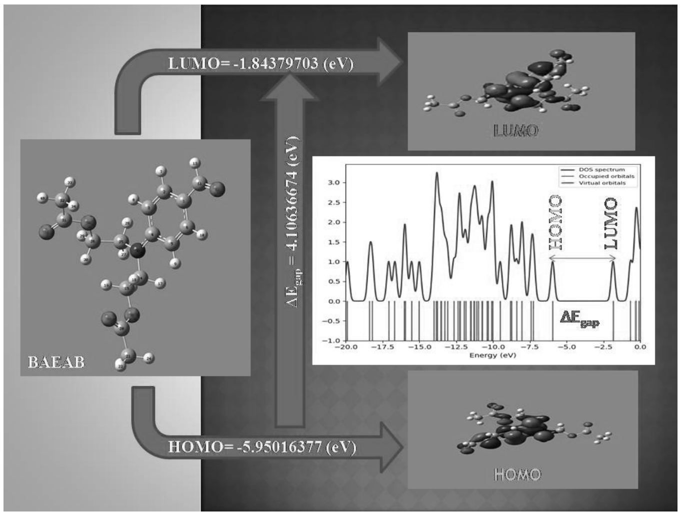

In this paper, the authors deals the theoretical investigation of molecular structure scan (Z-matrix) geometry optimization, global and local chemical reactivity descriptors calculations, NBO study and vibrational wave numbers of the novel 4-[Bis[2-(acetyloxy)ethyl]amino]benzaldehyde (BAEAB) were carried out by DFT (B3LYP and B3PW91) methods with 6-31+G (d, p) basis set in water solvent. The calculated vibrational wave numbers are found to be in good agreement with experimental FT-IR spectra and PED analysis using VEDA 4 program. The UV-Vis absorption spectrum of BAEAB was calculated by using TD-DFT/B3LYP/6-31+G (d, p) in gas phase, water, chloroform, DMSO and DCM solvent using CPCM model and λ_{max} in range of 354.16 nm, 341.35 nm, 343.74 nm, 342.18 nm and 342.64 nm respectively. The density of state (TDOS spectrum) of the compound in term of HOMOs and LUMOs and MESP were calculated and analyzed. The temperature effects on thermodynamic properties are discussed. The calculated ^{1}HNMR and ^{13}CNMR chemical shift using GIAO method and solvent effect are investigated by B3LYP/6-31+G (d, p) in gas phase, chloroform, water, DMSO and DCM solvent and correlate with experimental spectra. The dipole moment, polarizability and the first static hyperpolarizability values show that the BAEAB molecule is active nonlinear optical (NLO) material. The nucleophilic and electrophilic reactive sites in the BAEAB are analyzed by Fukui function analysis using mulliken charge. The charge transfer, conjugative interactions and delocalization of electron density are analyzed by natural bond orbital (NBO) analysis. The biological properties of BAEAB are also discussed.

Keywords: BAEAB, DFT/TD-DFT, Spectroscopic Data, NLO, NBO, Fukui Function Analysis

OP-15

Changing Climate and its Impact on Developing Countries

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The changes based on Industrial Revolution, together with the developments in science and technology have resulted in the increase in the world population. This has led to enhancement in anthropogenic greenhouse

gas emissions and concerns for human welfare. Such changes have caused the composition of the atmosphere to vary. This has created a change in the global climate. According to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change, this change will severely diminish the impact of the struggles for sustainable development.

In order to reduce greenhouse gas emissions, global mean surface air temperature needs to be reduced over the course of the next few decades. Another aspect which is helpful in the mitigation of climate change is reduced black carbon (BC, soot). BC has a strong positive radiative forcing in the atmosphere. The decline in surface air temperature with reduced BC emissions is weaker than would be expected from the magnitude of its instantaneous radiative forcing at the top of the atmosphere (TOA).

The present discusses the major issues that are helpful in mitigation of changing climate scenario of a developing country like India.

OP-16

Kinetic, Spectral and DFT Study of Oxidation of Diclofenac Sodium by Sodium Periodate

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Diclofenac, a widely used anti-inflammatory drug, has been found in many sewage treatment plant effluents, rivers and lake waters, and has been reported to exhibit adverse effects on fish. The kinetic of the degradation reaction and the nature of the intermediate products were still poorly defined. The kinetics and oxidation of diclofenac sodium (DFS) by sodium periodate in alkaline medium at 303 K and at a constant ionic strength of 0.60 mol dm^{-3} were studied iodometrically and spectrophotometrically. The effect of added products, ionic strength and dielectric constant of the medium was studied. The oxidation reaction in alkaline medium has been shown to proceed via a complex formation, which further reacts with one molecule of IO_4^- in a rate determining step followed by other fast steps to give the products. The reaction between DFS and $NaIO_4$ in alkaline medium exhibits 1:2 stoichiometry. The catalytic constant (K_c) was also calculated for proposed reaction at different temperatures and values of activation parameters with respect to the catalyst have been evaluated from the Arrhenius and Eyring plots and thermodynamic quantities were also determined. The oxidation products were [2-(2, 6-dicloro-phynylamino) - phenyl]-methenol identified by UV and IR spectral studies. The active species of catalyst and oxidant have been identified. From enthalpy-entropy relationships and Exner correlations, the isokinetic temperatures (333 K and 326 K) have been determined for the reactions. Proton inventory studies in H_2O - D_2O mixtures have shown the involvement of a single exchangeable proton of OH^- ion in the transition state.

Keywords: Kinetics, Oxidation, Diclofenac Sodium, $NaIO_4$, Os(VIII) Catalysis

OP-17

Spectroscopic and Kinetic Study of Formation of $[Ru(Cn)_5inh]^{3-}$ Complex on Aqueous Medium

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The present study deals with the synthesis and kinetics of $[Ru(CN)_5INH]^{3-}$ complex formation by substitution of cyanide ion in $[Ru(CN)_5H_2O]^{3-}$ anion by isoniazid (Pyridine-4- carboxylic acid hydrazide) [INH] ligand. The kinetics of reaction has been monitored spectrophotometrically in aqueous medium, by measuring an increase in absorbance at 502 nm (λmax of the light yellow coloured complex), which corresponds to the metal to ligand charge transfer (MLCT) transition, due to the formation of the final substituted complex $[Ru(CN)_5INH]^{3-}$. The synthesized complex $[Ru(CN)_5INH]^{3-}$ was characterized by ^1H and ^{13}C nuclear magnetic resonance, infrared and mass spectral analysis. The presence of a strong absorption bands at 3049.46 cm^{-1} and 3014.74 cm^{-1} for asymmetric and symmetric stretching vibrations respectively, shows the presence of a free amino (NH_2) group. The ESI-mass spectrum of the formed complex shows a molecular ion peak, [M+H], at m/z = 365.00, which confirms the stoichiometry of the complex formed. Thermodynamic and kinetic parameters have also been computed, using Eyring and Arrhenius equations and values of E_a, $\Delta H^{\#}$, $\Delta G^{\#}$ and $\Delta S^{\#}$ were found to be 49.8 $kJmol^{-1}$, 47.3 $kJmol^{-1}$, -8.62 $kJmol^{-1}$ and 187.6 $JK^{-1}mol^{-1}$ respectively. The reaction was found to obey first order kinetics with respect to [INH]. A most plausible mechanistic scheme has been proposed based on experimental findings.

Keywords: Kinetics, Hexacyanoruthenate(II), Isoniazid(INH) Ligand Substitution Reaction, Spectroscopy

OP-18

Studies of Bi-ionic Potential of Barium Molybdate Model Membrane

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The parchment supported model membrane was prepared by the ion-intraction method. The Bi-ionic potential (BIP) of model membrane bathed in different concentration of uni-univalent electrolytes (KCl, NaCl and LiCl) have been measured. Theoretical value of BIP have been calculated using the BIP theories developed recently by Toyoshima et al based on principles of non equilibrium thermodynamics. Comparison of experimental and theoretical BIP Values shows that theoretical equations of BIP are applicable to the model membrane. The model membrane have been characterized on the basic of TGA, DSC, TEM, SEM, FTIR and XRD analysis.

OP-19

Impact of Green House Effect on Vegetable Production

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The greenhouse effect is defined as when the Earth's atmosphere becomes thick with gases and substances which trap the sun's radiation, making the Earth warmer. An example of the greenhouse effect is global warming. The greenhouse effect is a process that occurs when gases in Earth's atmosphere trap the Sun's heat. This process makes Earth much warmer than it would be without an atmosphere. The greenhouse effect is one of the things that make Earth a comfortable place to live. Greenhouse effect is very important for all living beings. It's only the greenhouse effect which has maintained the temperature of earth. A greenhouse gas is a gas in an atmosphere that absorbs and emits radiant energy within the thermal infrared range. This process is the fundamental cause of the greenhouse effect. The primary greenhouse gases in Earth's atmosphere are water vapor, carbon dioxide, methane, nitrous oxide, and ozone

Greenhouse effect, a warming of Earth's surface and troposphere (the lowest layer of the atmosphere) caused by the presence of water vapor, carbon dioxide, methane, and certain other gases in the air. As Earth's surface is heated by sunlight, it radiates part of this energy back toward space as infrared radiation. Greenhouse vegetable production has traditionally been located near population centers, primarily in the northeastern States. Improved transportation and high energy costs have forced the industry south. With light being one of the most important factors in greenhouse vegetable production, the Southwest has become an ideal area for future development of this industry, particularly in the winter months when tomato and cucumber prices are at a premium. The crop production sector is responsible for CO_2 emissions both directly, depending on soil management practices, and indirectly, through the consumption of intermediate goods (fuel, etc.). The emissions of GHGs results in acid rain and earth's temperature rise (global warming). The destabilization of the global climate destroys natural ecosystem and increases natural disasters, such as violent storms, floods, droughts etc. The acid rain and these natural disasters affect the vegetable productivity. Yield is often higher as well, if you can provide optimum growing conditions for each crop. Greenhouses protect crops from many diseases, particularly those that are soil borne and splash onto plants in the rain. And greenhouse crops may be protected from common field pest.

OP-20

A Greener Approach towards Synthesis of Therapeutically Important Molecules

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Billions of people die due to various health ailments like pathothogenic or lifestyle diseases every year worldwide. The development of resistance and multidrug resistances in pathogen make this situation more critical and crucial. So the Scientists and Chemists involved in drug discovery research and Medicinal Chemistry programme have tremendous burden of developing new therapeutics to combat this situation. As a result a number of new synthetic molecules are being synthesized everyday in order to get molecules of better biological property. This creates huge environmental trouble as the conventional chemical synthetic protocols end with hazardous chemicals and by products to pollute the environment. Therefore, there is urgent need to develop environmentally benign and green synthetic protocols for synthesis of therapeutically important molecules or nucleus. These situations lead to the development of various methods like using Green Solvents, Green Catalysts. During last decade organic reactions In water and On water presented some better alternatives for organic chemists to develop sustainable protocols. Apart from water as solvents several other green solvents as Poly Ethylene Glycol (PEG) and supercritical fluids used as green solvents. Some environment friendly organocatalysts as L-proline and supramolecular catalyst as β-cyclodextrins were also exploited green catalysts for synthesis of small heterocyclic molecules. Ultrasound Medium, Microwave reaction medium and some other synthetic procedures also proposed some better alternative methods for green synthesis. Reactions in Ionic liquids also emerged as a greener way to perform synthetic chemistry. Microwave mediated organic synthesis provides an easy and green alternative for the synthesis of small organic molecules. In order to develop greener and sustainable protocols for synthesis of small molecules in multicomponent manner we utilized these alternatives methods and reported few environmentally benign synthetic methodologies for indole based heterocycles. In present work I discussed the need of green and sustainable chemistry and our work in respective field. I will talk about the role of green solvent, green catalyst and use green protocols for synthesis of small molecules of therapeutic interest.

OP-21

Perovskite Structured Nanomaterials as the Advanced Key for Global Development of Nanotechnology

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Perovskite structured nanomaterials had originated from CaTiO3. They are a class of compounds with the general formulae ABX3. Now a day they are on the centre of focus including very important family of materials. Perovskite type metal oxide nanomaterials exhibit a wide range of ferroelectric, piezoelectric, and pyroelectric properties along with numerous opto-electrical effects. They have been using as electronic, structural, magnetic and refractory materials in numerous technological applications. Including many applications, the effective photocatalytic activity can be attributed to the spatial structure of perovskite. After all, the structural features for designing the perovskite type metal oxide nanomaterials give a possibility to use almost 90% of the metallic natural elements of the periodic table and often find the way to correlate the solid state chemistry to photocatelytic activities. Nanoparticles (NP) are applying rapidly for global development because of their higher responsiveness and degree of function, large surface area, size-dependent properties etc.

Keywords: Nanoparticles, Perovskite Structure, Catalyst, Global Nanotechnology

OP-22

Synthesis of Silver and Gold Nanocomposites and their Effective Cytotoxicity Against Lung Cancer A-549 Cells

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The beginning of the global era has demanded the scope of material sciences including the synthesis of nanoparticles to diagnose a number of ailments in vitro analysis. Silver and Gold nanocomposites have been prepared by sonochemical methods to propose their coordinate complexes from their salts. The formed nanocomposites have been used for the cytotoxicicity study, effective against human carcinoma cells A-549. The formed nanocomposites have been used for their immunoassay against therapeutic purpose, antimicrobial and antifungal too. Spirillum, Rod shaped Ag-Au Nanoparticles(Ag-AuNP) have been synthesized using L-Ascorbic Acid with an ambiphilic nonionic surfactant(PEG) via the sonochemical method. The shape size and the distribution of the formed nanoparticles have been tuned by changing the reduction temperature, resulting evolvement of uniform Ag-AuNP with a size of 8.52 nm or 21.03 nm. The facets of the have been investigated by the high resolution electron microscopy. The cytotoxicity of the Ag-AuNP have investigated through human lung cancer cells(A-549) at 37°C, and the biological adaptability exhibited by Ag-AuNP has opened a pathway to biochemical and biocatalytic application such as drug-delivery system, photochemical treatment and biosensors and immunological response too.

Keywords: Nanocomposites, Spirillum, Ag-AuNPs, L-Ascorbic Acid, Polyethyleneglycol

OP-23

Bioremediation: A Ultimate Technique for Sustainable Development; Review Article

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Bioremediation can be defined as any process that uses microorganisms or their enzymes to return the disturbed environment to its original condition. It has the potential of complete degradation or transformation of hazardous organic pollutants into harmless products. During the process of bioremediation, nutrients are added

to the contaminated area in order to stimulate the growth of the appropriate microorganisms, which accelerates the biodegradation of the polluting toxin. Bioremediation can take place in two conditions that are aerobic and anaerobic conditions. In anaerobic condition, microbes need oxygen to perform their duty. Bioremediation relies on stimulating the growth of certain microbes that use contaminants like oil, solvents, and pesticides as a source of food and energy. These microbes consume the contaminants, converting them into small amounts of water and harmless gases like carbon dioxide. Bioremediation can either be done in situ, at the site of the contamination itself, or ex situ, at a location away from the site. The process of bioremediation can take anywhere from a few months to several years. Finally, bioremediations is cheaper than most clean up methods, as it does not require a great deal of equipment or labour. As of 2012, bioremediation has been used to clean up more than 100 Superfund sites around the United States.

Keywords: Bioremediation, Anaerobic, Aerobic, Intrinsic Bioremediation, Bio-augmentation, Microorganism, Bio Stimulation

OP-24

Experimental, Molecular Docking and DFT Studies of Zn(II) Complex of S-benzyl β-(N-3-(2-nitrophenyl)Allylidene) Dithiocarbazate as Biologically Active Agent

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The NS based S-benzyl β-(N-3-(2-nitrophenyl)allylidene)dithiocarbazate (HL) Schiff base was synthesized by 1:1 condensation method between S-benzyl dithiocarbazate and trans-o-nitro cinnamaldehyde. The structure of the compound was elucidated by FT-IR, Mass, ^{13}C-NMR, Raman, ^{1}H-NMR, and UV-Vis both by spectroscopic and computational techniques. Computational docking studies were carried out to identify the biological targets. The binding energy for DNA and proteins (3C5W) were -19.6648 and -20.5016 kj/mol and the adducts were stabilized by H-bonding and hydrophobic attractions. Its anti-bacterial activity is assayed against two commonly infection causing bacterial strains namely gram-positive *S. aureus* and gram-negative *E. coli*. The results showed appreciable biological activity and the activity increased with increase in concentration. Thermal stability of the ligand was carried by TGA up to 500 ^{0}C, decomposes fully to give gaseous products. Theoretical investigation of HL has been accomplished using DFT- B3LYP quantum chemical method in combination with B3LYP exchange correlation functional. VEDA-4 (Vibrational energy distribution analysis) software was employed for theoretical FT-IR spectrum analysis which yielded 111 fundamental vibrational modes along with potential energy distribution percentage (PED%) showing non-linearity of HL. Theoretically calculated parameters like UV-VIS, FT-IR, ^{1}H-NMR, ^{13}C-NMR, Raman, HOMO-LUMO energy gap and electrostatic potential were in conformity with calculated results.

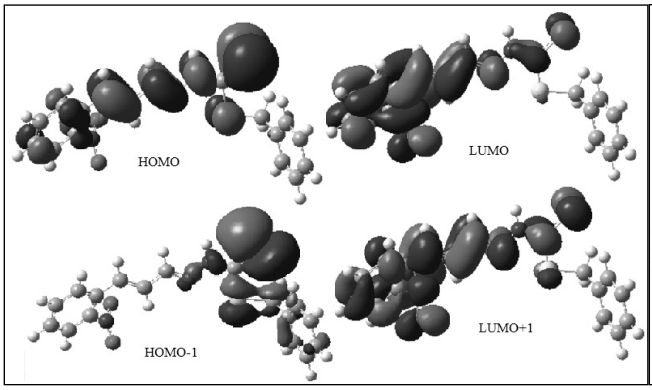

Fig. 1: 3D Plots of Frontier Molecular Orbitals of H

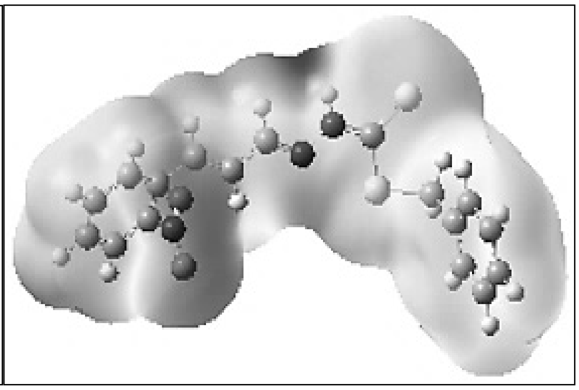

Fig. 2: MEP by B3LYP/6-311++G(d,p) Level of HL

OP-25

Study of First hyperpolarizabiliy and Intermolecular Interaction of N-(substituted)-2-[4-oxo-2-Phenylquinazolin-3(4H)-yl] Acetohydrazide Derivatives through DFT Approach

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A series of novel N-(substituted)-2-[4-oxo-2-phenylquinazolin-3(4H)-yl] acetohydrazide derivatives were designed and synthesized, and their structures were characterized by ^{1}H, ^{13}C NMR, IR and Mass Spectral analysis. All experimental spectral data good overlay with theoretical data. The theoretical data were calculated by using B3LYP functional with 6-13G basis set through Guassian 09 Program. The first hyperpolarizabilty value indicates that synthesized compound is used in optical switching, optical modulator material etc. Intermolecular interaction was seen by AIM program.

Keyword: Quinazolinone, Schiff Base, NMR, IR, Mass Spectra, NLO, AIM

OP-26

Synthesis of 2, 3-diaryl Benzofuran Derivatives by Incorporating Greener Steps: An Approach for Sustainable Development

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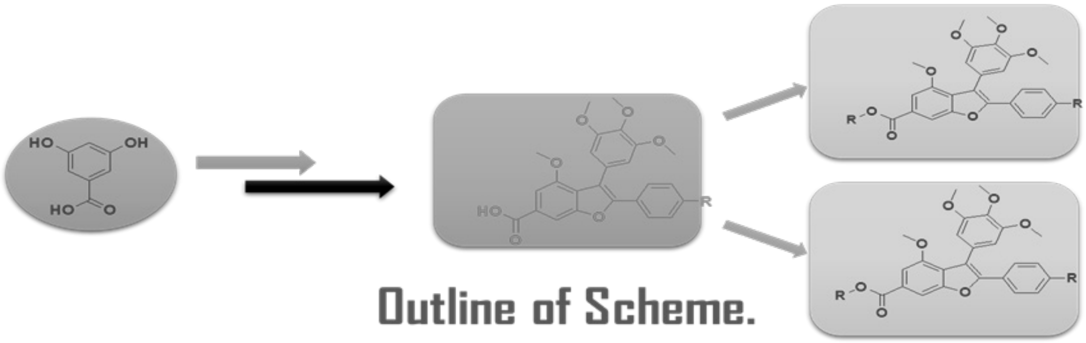
Palladium-catalyzed cross coupling reactions are indispensable tool in organic synthesis with numerous applications in medicinal chemistry and natural products synthesis. The 2, 3-diaryl benzofuran was synthesized by utilizing a three step-sequence consisting of Sonagashira coupling, Iodocyclization and Suzuki coupling reactions. Further, 2, 3-diaryl benzofuran was modified to seventeen new derivatives and were in-vitro evaluated for their antitubercular potential. Among all, four derivatives showed antitubercular activity in the range 12.5 – 50 μg/mL. From this study it was observed that the derivatives containing halogen moieties possessed higher antitubercular activity while trimethoxy group showed lower activity. Apart from the above, 2, 3-diaryl benzofuran derivatives also showed anticancer activity against the various human cancer cell lines

Introduction: Tuberculosis (TB) is a contagious air-borne bacterial disease caused by the infection from Mycobacterium tuberculosis (Mtb) affecting mainly lungs. Over the period of time, the pathogen has become resistant to two most powerful drugs like rifampicin and fluoroquinolones. To tackle this situation, there is a need to explore for new anti-TB molecules.

Methods: The synthesis of 2, 3-diaryl benzofuran was synthesized by utilizing a three step-sequence consisting of Sonagashira coupling, Iodocyclization and Suzuki coupling reactions. Further, 2, 3-diaryl benzofuran was modified to seventeen new derivatives

Results: Synthesis of 2, 3-diaryl benzofuran achieved and seventeen derivatives prepared among all, four derivatives showed antitubercular activity in the range 12.5 – 50 μg/mL

Discussion: The 2, 3-diaryl benzofuran was synthesized by using green chemistry approach. Four derivatives show significant antitubercular activity. Among four derivatives compound-BALTSRU-115 was very potent. Detailed mechanistic/target studies of antitubercular activity will be discussed in the Global Conference



Outline of Scheme.

OP-27

Design, Synthesis of Sugar based Surfactants and Studying their Physicochemical Properties

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The synthesis and characterization of sugar-based surfactants derived from sugar and amino acid. Physico-chemical properties, such as solubility and melting points, and surfactant properties, like, dispersion, emulsification, and foaming were investigated.

A number of sugar based surfactants was synthesized from sugars and amino acid compounds. Monosaccharide's, (D-glucose, 2 -deoxy-2-amino-D-glucose) fructose and D-(+)-glucono-1,5-lactone, were used for the hydrophilic surfactants. The hydrophobic moiety consisted of fatty acids and long chain alkyl groups, as well as aromatic compounds. In general, the synthetic procedures gave high yields in few steps. Some novel surfactants were prepared in high yields in simple synthetic step.

The general structure-property relationship of the surfactants since no clear trends could be observed. All surfactant properties were compared to those of common commercial surfactants. The aqueous solubility follows the general trend expected from the HLB of the surfactant when considerations about the character of the head group and the connecting unit are added. Some surfactants were able to form macro emulsions between water and different oils. The emulsions were stable for several months. Surfactants with open sugar head groups, in contrast to closed sugar head groups, were found to be better dispersion agents. Increasing the size of the tail group, by using twin chain tail groups, increased the dispersion properties further. The wetting properties of the sugar-based surfactants were generally found to be poor. Foaming properties were low for surfactants with low aqueous solubility.

Keywords: Surfactants, Surface Properties, Melting Point, Foaming, Dispersion, Emulsification, Solubility

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OP-28

The Prospects of Green Energy Policies in India

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Renewable energy sources and technologies have potential to provide solutions to the long-standing energy problems being faced by the developing countries. The renewable energy sources like wind energy, solar

energy, geothermal energy, ocean energy, biomass energy and fuel cell technology can be used to overcome energy shortage in India. India is increasingly adopting responsible renewable energy techniques and taking positive steps towards carbon emissions, cleaning the air and ensuring a more sustainable future. Developing nations are now driving the world's gradual shift towards renewable energy, and India has become one of the leaders of the pack. With the right investments in green technologies, India is well positioned to achieve renewable energy targets. The pursuit towards cleaner energy will have a crucial role in enabling the country's transition to a fully sustainable energy system. With increased investments and clean energy installations, as well as the world's largest renewables auction market, India ranks 2nd after Chile in the 2018 Climate scope report by energy researcher Bloomberg NEF. The organisation studied over 80 indicators, such as clean energy policies, power sector structures, emissions and installed capacities, for 103 countries around the world. India's second position represents a climb of three spots from the 5th position it held last year. In comparison, China ranked 7th, down from the top position last year.

Methods- A doctrinal and analytical approach has been adopted to evaluate critically the progress of India in terms of Green Energy.

Results and Discussion- In this paper, efforts have been made to summarize the availability, current status, major achievements and future potentials of renewable energy options in India. This paper also assesses specific legal and policy interventions for overcoming the barriers so that necessary changes can be made in the policies to enhance deployment of renewables for the future.

OP-29

Humidity Detection Ability of the Graphene Oxide Functionalized with the Iron Nanoparticles

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Chemical wet method is used to functionalize the Graphene oxide (GO) with iron nanoparticles. The SEM, EDX, BET, XRD, FTIR, UV Vis spectroscopy and Raman characterization techniques are employed to characterize the synthesized materials. These characterization techniques confirmed the iron nanoparticles are attached to GO at the oxygen containing functionalities present in within it. The synthesized GO functionalized with iron nanoparticles (Fe-GO) is implemented for the humidity sensing because of high porous morphology and dangling bonds present in the material.

Keywords: Graphene Oxide, Functionalization, Humidity, Iron Nanoparticles, Sensors

OP-30

Electrophoretically Deposited Nickel-Boron Nitride Coatings: An Advanced Material for Environment Protection

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Nickel with chemically and thermally stable hexagonal boron nitride (Ni-BN) is used as dry lubricant coating for high technology applications of automotive and aeroengines. The release of hydrocarbon pollutants, motor oil and hydraulic fluid after an aircraft crash cause soil and water pollution. Herein, in order to protect aircrafts damage and thus our environment, electrophoretically deposited Ni-BN composite coating was strengthened with graphene (Ni-BN-Gr), carbon nanotubes (Ni-BN-CNT) and diamond (Ni-BN-D) carbonaceous reinforcements. Highest hardness (2.0 GPa) and elastic modulus (133.5 GPa) of Ni-BN-D coating than Ni-BN-CNT (1.96 GPa and 102.1 GPa respectively), Ni-BN-Gr (1.94 GPa and 92.0 GPa respectively) and also from Ni-BN (1.89 GPa and 91.5 GPa respectively) coatings was linked through high compressive stress (-601 MPa), dislocation density (8.9 1015 m-2) and yield strength (4.4 GPa), calculated by Taylor's model. Addition of graphene, CNT and diamond in Ni-BN composite showed a decrease in wear volume (from 1.66 10-8 m3 to 0.45 10-8 m3) due to the synergetic lubricating effect of BN and carbonaceous reinforcements. The friction mechanism during micro-scratching was predicted by friction model and the contribution of ploughing and adhesion components was compared with the experimental frictional values. Thus Ni-BN-D restrict inception of multiscale wear and can be a potential three phase metal-ceramic coating for engineering, industrial and environmental applications.

OP-31

Exploring the Potential of Jhingan Gum for Diverse Applications: A Review

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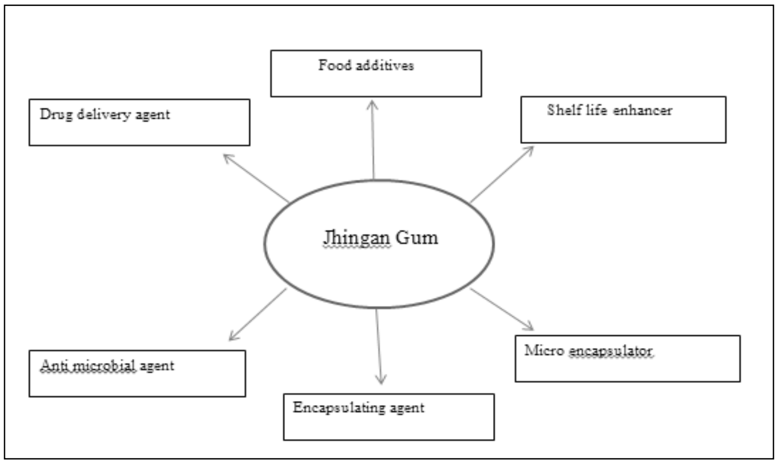
Large number of plants exudate complex polysaccharides as a consequence of mechanical/micro-biological injury. Exudates of gums are always in high demand for usage as food additives, emulsifiers and other applications and in pharmaceutical field as they are non-toxic, economically viable, readily available and are safe enough for human consumption. Many species of exudate gums have been reported to have therapeutic application and Jhingan gum is one of them. Jhingan gum is classified as Arabino-galactan, similar to Gum Arabic, is an unexplored minor gum. Different aerial portions of the plants are used in varied ways in medicinal field. The plant is reported to contain gums and mucilages which yields Arabino-3,6-galactan on hydrolysis. It contains L-rhamnose with 2.5%, L-arabinose with 11%, 4-O-methyl uronic acids with 17% and D-galactose being the major portion with 69.5 %. The gum also yields 1.38% of Proteins. Since this gum is similar to Gum Arabic and is not yet extensively used, it remained unexplored in the field of agriculture and in industries such as textiles, paper, cosmetics, drug delivery, confectionaries and pharmaceuticals. This article would serve as a base for biopolymer studies leading to commercialization of Jhingan gum in various applications.



Keywords: Jhingan, Natural Gum, Minor Gums, Plant Products

OP-32

Purine Based nucleoside Analogues Developed as Anticancer Drugs

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Nucleoside analogues represent an important class of scaffolds in anticancer drug discovery for many years [1]. We have synthesised a novel series of purine based scaffolds and their bio-evaluation as an anticancer agent. The structural gratitude of anticancer nucleoside analogues by cellular enzymes depends on the hydroxymethyl group for phosphorylation, heterocyclic base responsible for the hydrogen bonding, and the sugar moiety as a spacer connecting the hydroxymethyl group and the nucleobase in the proper orientation. Marketed drugs have showed unlimited benefits in the treatment of breast cancer, however, resistance restrict their use [2]. The rational designing of multi-target drugs can reduce side effects and increase the tolerance of anticancer agents. In this work, a series of 2-amino-6-chloropurine based glycoconjugates derivatives were designed and synthesized to target VEGFR.

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OP-33

Determination of Urinary PAH Metabolites using DLLME Hyphenated to Injector Port Silylation and GC-MS/MS

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Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous environmental pollutants and well known carcinogens. PAHs are considered as biomarkers of PAH exposure and there is a need to measure these metabolites at low concentrations. So, an effective, easy, precise and eco-friendly analytical method has been developed for rapid determination of PAH metabolites. New analytical method which is first time introduced, based on coupling of dispersive liquid-liquid microextraction (DLLME) with auto-injector port silylation (auto-IPS) followed by gas chromatography-tandem mass spectrometry (GC-MS/MS) analysis is reported for the analysis and quantitative determination of urinary PAH metabolites. The factors affecting method, such as type and volume of extraction and disperser solvent, pH, ionic strength, injector port temperature, volume of N,O-Bis (trimethylsilyl) trifluoroacetamide (BSTFA) and type of solvent were inspected. Under optimized conditions, the limit of detection and limit of quantification were found to be in the range of 1–9 and 3–29 ng mL-1 , respectively. Very good recoveries of metabolites in urine samples in the range of 87–95% were found. The analytical method has been applied for the quantitative determination of PAH metabolites in urine samples of exposed workers. The developed method (DLLME-auto-IPS-GC-MS/MS) is time, labor, toxic solvent and chemical saving, which can be routinely applicable for the analysis of urinary PAH metabolites of human samples.

Keywords: Dispersive Liquid-Liquid Microextraction, Injector Port Silylation, Polycyclic Aromatic Hydrocarbon Metabolites, Gas Chromatography-Tandem Mass Spectrometry

OP-34

Carbene Catalyzed Stetter Reaction: Synthesis of Phosphonate 1,4-Diketone to Access Phosphonate Containing Heterocyclic Compounds

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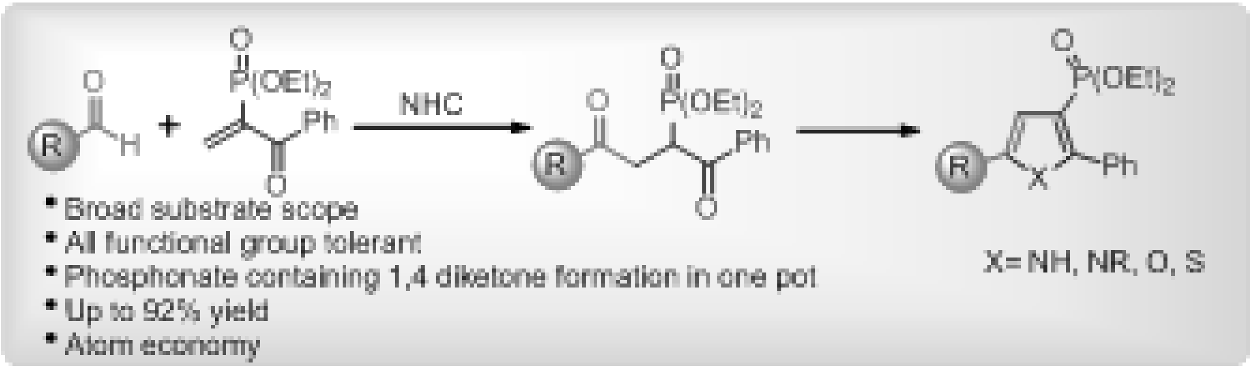

Organophosphorus compounds are an important class of molecules which has potential applications in materials chemistry, pharmaceuticals, agrochemicals, and in catalysis. Therefore, the catalytic synthesis of phosphonate/ phosphate containing 1,4-dicarbonyl compounds in a concise manner is a highly desirable and challenging endeavor in organic synthesis. To the best of our knowledge, there is no report on metal-free Stetter reaction for the synthesis of phosphonate containing 1,4-diketone.

Here in, we report the first carbene catalyzed Stetter reaction of aldehydes and enals with β-unsubstituted vinyl ketophosphonate for the synthesis of phosphonate containing 1,4-diketone. The products were obtained in good to excellent yield with wide substrate scope. These 1,4-diketone could be converted to the various phosphonate-bearing heterocycles compounds like thiophenes, furans and pyrroles.

OP-35

Kinetics of Complex Formation of Fe(III) with Gallic Acid: Experimental and Theoretical Study

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Kinetic study on the complexation of gallic acid with ferric chloride was performed in aqueous solution at pH 8.0. The complex was characterized by IR, UV-Vis spectroscopy and FE-SEM techniques. Kinetic data were obtained and used to model the reaction kinetics for the disappearance of the gallic acid. The operational variables have been studied in the temperature range from 25 to 45°C. The complexation reaction was found to obey a first-order kinetics with rate constants for k1 (formation) 3.7×10-3 sec-1. Additionally, the effect of concentration and temperature on the complexation reaction was investigated. Apparent kinetic parameters of the complex formation of Fe(III) with gallic acid were found as; pre-exponential factor [A = -1.17 min-1], enthalpy of activation [(ΔH°)# = -2278 J mol-1], entropy of activation, [(ΔS°)# = -6.34 J mol-1 K-1] and Gibbs free energy of activation, [(ΔG°)# = -0.57 J] . The apparent activation energy of the complexation reaction was evaluated to be 273.29 J mol-1 which is consistent with the chemistry of Fe(III) with polyphenols which are supposed to mimic the interaction of Fe(III) with transferrin in biological media. Various theoretical parameters of the studied complex such as hardness, electronegativity, softness, total energy, dipole moment and point group symmetry were calculated employing Density functional theory (DFT) and found as 0.03465, 0.2230, 21.39, 0.5101×10-8 eV, 16.13 Debye, and C1, respectively.

Keywords: Fe(Iii), Gallic Acid, Complex, Kinetics, Apparent Kinetic Data, DFT

OP-36

Industrial Development: Ozone Layer Depletion and Its Consequences

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Modernization of life style would directly and indirectly impact on environment. India is a developing nation as well as biggest economic centre in the world that create unsound following problems such as Industries emit harmful gases which increases the air pollution while there Industrial wastes are discharged into the rivers create water problems. There are many situations where human activities have significant effects on the environment.

Ozone layer damage is one of them because it prevents the penetration of UV and high energetic rays into the atmosphere. But due to extensive industrialization it is damage and there is hole created over the Antarctica, Australia and other part of world too. Here we would discuss the impact of ozone holes and its consequences.

Keywords: Industrialization, Environment, Ozone Layer & Hole

OP-37

Integrated Approach of Nanotechnology: Low Temperature Synthesis of ZnO Nanowires and its Application Over Dye Discoloration Reaction

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Nanotechnology representing a new frontier in modern science and technology and is anticipated to become a major thrust in near future by offering potential applications. Afterward 1970s industrial boom; the textile, paper and other industries are directly associated with disposal of large number of different toxic pollutants, those are not only harmful to the aquatic environment but also hazardous to human health as they are non-biodegradable. Recently, National Institution for Transforming (NITIAayog) India; published a report that there would be scarcity of water supply throughout the India after 2025. So, it is clarion call to check out the industrial effluents and recycle the water for further use.

There were various different methods has been used for cleaning of industrial effluents but among them heterogeneous photocatalysis is an advanced oxidation process because of following reasons, it is extensively employed;

√ They are inexpensive.

√ They show low or no toxicity.

√ They show substantial stability and durability.

and provided an indifferent path to achieve remarkable results.

The as-synthesized ZnO nanowire posses high aspect ratio were exhibited remarkable results for photocatalytic degradation of Rhodamin-B under UV-light illuminations.

Keywords: Nanomaterials, XRD, FESEM, UV-Vis, P.L & Photocatalysis

OP-38

Asymmetric Oxidative Rearrangement/ Functionalization of Olefins Using Hypervalent Iodine

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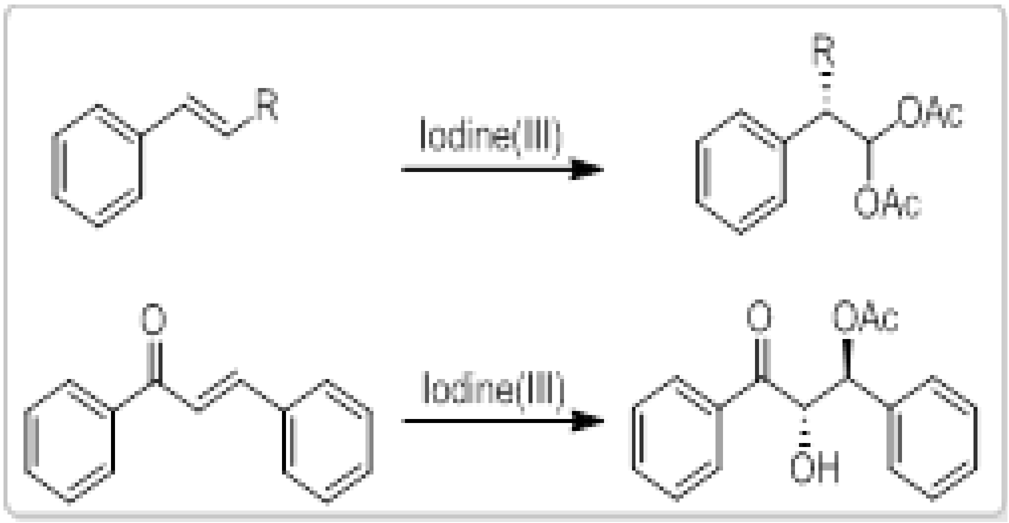

Hypervalent Iodines have emerged as an alternate and sometimes even superior mode of catalysis over toxic metal-based catalysts due to their inherent environmentally benign reaction condition and diverse reactivity. Hypervalent Iodines prominently work as an oxidant but their reactivity is not limited only to these oxidative properties. They catalyse many reactions through activation of olefins towards various nucleophilic additions. Besides these, they also propagate different kinds of rearrangements on the substrates.

Here in, we report a stereoselective oxidative rearrangement of β-substituted styrenes to give α-aryl substituted diacetate in good to moderate enantioselectivity employing chiral I(III)- reagents. A DIBAL-H mediated reduction these products produced the corresponding chiral α-aryl substituted alcohols.

In addition, we have also achieved the first enantioselective mono-hydroxylation-acetoxylation of chalcones using hypervalent iodine reagents. The literature known methods for the dihydroxylation of alkenes requires highly toxic metal-based catalysts like OsO4/RuCl3/CeCl3/NaIO4. These all produced racemic dihydroxy deriavtes in the absence of chiral ligands, not acetocy-hydroxylated products. The mono-protected dihydroxy derivatives obtained in this study allows for easy manipulations of each hydroxyl-group. All the products were obtained in good to excellent enantioselectivity and yields. The reaction condition tolerates many labile groups.

OP-39

Environmental Benign Synthesis and Characterization of Argentum Nanoparticles and its Biological Application

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In the present paper nanoparticles was synthesized by using egg-white as a bio-reducing agent. The protein of egg-white, which have different functional groups displayed important routes in reducing Ag^+ ions and maintaining stability and dispersity. Synthesized silver nanoparticles was characterized, using UV-Vis spectrophotometer, Field Scanning Electron Microscope (FESEM), Transmission Electron Microscopy (TEM), Fourier transform infrared spectroscopy (FT-IR) and X-Ray Diffraction (XRD). The morphology and particle size of Ag NPs are obtained by FESEM, TEM and XRD. The TEM analysis confirmed the spherical shape of obtained Ag NPs. The XRD pattern of synthesized AgNPs showed broad peaks, which confirm the nanocrystalline nature of Ag_2O. The particle size of the ZnO NPs is calculated by Scherer formula-

$$D = 0.9\lambda/\beta \cos\theta$$

where - D is the crystallite size, λ is the wavelength of radiation used, θ is the Bragg angle and β is the full-width at half-maximum measured in radian.

The results obtained indicated the formation of silver nanoparticles having uniform shape and particle size. The synthesized nanoparticles exhibit a well known pattern as observed by analysis it through size analyzer.

Keywords: Biological Application; Ag Nps; TEM; FESEM

OP-40

One-Pot Synthesis of Non-activated Aziridines

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Non-activated aziridines are present in many bioactive natural, synthetic and semisynthetic molecules; as well they also serve as versatile building blocks in organic synthesis[1]. They can undergo various transformations such as ring opening, ring expansion and rearrangements[2]. The syntheses of activated aziridines from olefins are well established while the direct methods for non-activated aziridines are less explored[3]. Herein we describe the highly efficient direct method for regio and stereospecific synthesis of Non-activated aziridines from olefins in a single step using O-(sulfonyl) hydroxylamine as the aminating agent, di-rhodium catalyst in 2,2,2-trifluoroethanol (TFE) as a solvent[4].

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OP-41

Microwave Assisted Synthesis of Acetamido-Benzoxazolone based TSPO Ligand for Positron Emission Tomography

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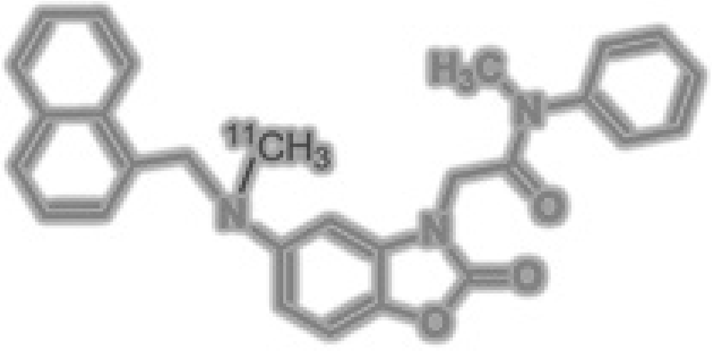

Introduction: The Translocator protein (18 kDa, TSPO) is an attractive target for diagnosis and treatment of several pathological conditions. Its up regulation has been especially reported in activated microglia of neuroinflammatory disorders such as multiple sclerosis as well in some type of cancers, including breast, colon and glioblastomas. The objective of the work undertaken is to synthesize TSPO ligand using green chemistry for application in Positron Emission Tomography (PET) post ^{11}C radiolabeling.

Methods: The synthetic strategy involves the cyclization of 2-aminophenol derivative using CDI in acetone for 20 min in microwave (mw) followed by alkylation utilizing 2-bromo-N-methyl-N-phenylacetamide. Further, nitro group on benzoxazolone derivative is reduced and alkylated with 2-(bromomethyl)naphthalene using K2CO3 in acetone for 40 min in mw leading to the formation of desired mono-substituted product, N-methyl-2-(5-((naphthalen-2-ylmethyl)amino)-2-oxobenzo[d]oxazol-3(2H)-yl)-N-phenylacetamide in 85% yield.

Computational docking and in-vitro binding studies were also performed to assess receptor binding efficacy of the ligand.

Results: The synthesis of acetamido-benzoxazolone derivative for Translocator Protein (18 kDa, TSPO) imaging is performed using green solvent under microwave conditions. Ligand is synthesized in high yield of 85% within short span of time with each compound verified by NMR, mass spectra and HPLC. Computational docking indicated towards higher receptor binding compared to previously well-known ligands. The in vitro binding affinity assessed on rat brain homogenates also confirmed the high binding of ligand for TSPO (K_i $=10.2 \pm 0.1$ nM) than central benzodiazepine receptor (CBR, K_i = >100 nM).

Conclusions: A novel acetamidobezoxazolone based derivative has been synthesized utilizing efficient, clean and economical synthetic strategy. Computational and in vitro analysis confirms higher receptor binding than formerly famous ligands. The advantage of developed TSPO PET ligand is its synthesis using green chemistry; high yield 85% with minimal solvent usage and short reaction time. In conclusion, derived ligand may serve as a promising marker for visualization of neuroinflammation via TSPO targeting using PET after labeling with ^{11}C.

OP-42

An Approach Towards One Pot Green Synthesis of 2,3-Dihydroquinazoline-4-(1H)-Ones using Isatoic Anhydride and EDTA

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Quinazoline is an important aromatic heterocyclic moiety which has two aromatic rings one benzene ring and other is pyrimidine ring. Quinazoline moiety is isomeric with quinoxaline, phthalazine, and cinnoline which are also aromatic heterocycle. Its derivative quinazolinone present in two isomeric forms, one is 2-quinazolinone and other is 4-quinazolinone are an important scaffold for various biologically important drugs as anticancer, antibacterial, antifungal, antimicrobial, ant inflammatory, ant analgesic, anticonvulsant agents, etc.

These moieties have been prepared by the different methods and a different molecule such as anthracitic acid, anthranilamide, 2-cyanobenzoic acid and isatoic anhydride in single and multiple steps. Isatoic anhydride is an important precursor for the preparation of quinazolinones in one pot synthesis using a different type of aldehydes with a different type of amines or ammonium acetate with or without catalysts and solvent. In the present study, we would like a report a new application of EDTA as an inexpensive, nontoxic and green catalyst for three component one pot synthesis of 2,3-dihydroquinazoline-4-(1H)-ones in water media. The methods seem to be a greener option as it is time saving reaction easy to handling and catalysts are recyclable. Herein presented is a ready reference for one pot synthesis of various quinazolinone molecules as an important drug intermediate from isatoic anhydride of the last 20 years.

Keywords: One Pot Synthesis, Isatoic Anhydride, Edta, Quinazoline, Quinazolinone, Etc

OP-43

Silver Nanoparticles Embedded Psyllium Nanocomposite: Green Synthesis, Characterization and Antibacterial Activity

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Psyllium/Silver nanocomposite (Psy/Ag-N-composite) was synthesized thoroughly in green way via simple in situ method by maltose sugar reduction using varying concentration of $AgNO_3$ solution. The synthesized composite was characterized by UV-vis spectroscopy, Fourier Transform Infrared spectroscopy, Scanning Electron Microscopy, Transmission Electron Microscopy and X-rays diffraction analysis. The synthesized composites were opted for antibacterial activity test performed by well disc diffusion method using tetracycline as reference drug. The Psy/Ag-N-composites were ascertained to exhibit outstanding antibacterial property against both gram-positive Staphylococcus aureus and gram-negative Escheria coli and Pseudomonas Aeruginos. It was found that the sample Dk1 exhibit maximum antibacterial activity among all synthesized composite samples against all of the applied pathogen strains.

OP-44

Alternative Uses of Sugarcane to Mitigate Green House Gases Generation

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The contribution of the sugarcane production, and, especially, of the sugarcane harvest system to the greenhouse gas emissions of the country is an issue of national concern. One of the significant avocations for bio-vitality frameworks is their low ozone depleting substance (GHG) discharges contrasted with fossil-vitality ones. Changing a sugar plant into a bio-vitality plant would add to environmental change relief by means of the extraction of sustainable power and ethanol. This examination takes the instance of the sugar business and recognizes situation alternatives that offer GHG decrease benefits. Improving effectiveness in power age from sugar stick deposits for example abundance bagasse and stick refuse is such a helpful alternative. Besides, extricating ethanol in a purported bio-refinery, where the coproduct stillage is used for vitality, will in general amplify the potential advantage. The biggest reserve funds potential accomplished with extricating ethanol from surplus sugar versus current practice in the sugar business adds millions of tons of CO_2 per year. This can't be

acknowledged practically speaking until the carbon obligation from land change is reimbursed, which takes 4– 7 years, expecting that the land changed over is meadow

However, a worry emerging with using nourishment crops for extended ethanol creation is land-use change from grassland or timberland to cropland. Whenever woods or field is cleared for new cropland, natural issue in vegetation and soil is discharged to the atmosphere as CO_2. This CO_2 discharge, whenever considered, may make the GHG execution of biofuels become more regrettable than that of customary petroleum derivatives. Using cane trash for vitality rather than open consuming in fields can acquire twofold advantages keeping away from uncontrolled discharges and making substantial GHG credit from power created to substitute for customary power generation in the national framework. Whenever isolated from the complete GHG investment funds, the commitment from the use of stick refuse is about 5.6 occasions that from the productive use of bagasse. Obviously, the more biomass-based power created, the more GHG outflows from customary fossil-based power plants maintained a strategic distance from and in this manner the more GHG reserve funds made.

OP-45

Synthesis and Characterization of Adsorbent using Power Ultrasound for the Evaluation of Specific Surface Area and Porosity: An Eco-Friendly Technique

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The aim of the present paper is to explain the comparative study of power ultrasound (PUS) assisted synthesized materials from agriculture waste materials for specific surface area and porosity. The use of an excess amount of chemicals during the preparation of adsorbent leads to uneconomical and also causes toxicity in the environment. This problem has received attention from several years, however, to date, there is no effective solution to get rid of this problem. The application of ultrasonication during the preparation of adsorbent avoids the excessive use of chemicals. Therefore, the present work focused on the preparation of adsorbent employing conventional impregnation and ultrasound-assisted impregnation (20 kHz). The synthesized adsorbents were characterized by attenuated total reflection Fourier transforms infrared spectroscopy (ATR FTIR), scanning electron microscopy (SEM), optical profilometry (OP), Brunauer–Emmett–Teller (BET) analysis and X-ray diffraction (XRD) techniques. The SEM, elemental mapping and nitrogen adsorption determined the active site dispersion. The SEM analysis illustrates the surface microstructural aspects of the adsorbent. The XRD analysis provides the crystallographic structure and grain size of adsorbent. The two important physical properties (specific surface area and porosity) that impact the quality and utility of solid phase materials, therefore, BET method was used to determine the surface area (S_{BET}) and porosity of the adsorbent. In BET analysis nitrogen and helium were employed as adsorbate and carrier gas respectively. The physical characteristics of porous material such as skeletal density (ρS), porosity, total pore volume (TOPV), and pore size distribution (PSD) was obtained from N_2 adsorption-desorption isotherm, PCI curve, BET plot, Langmuir plot, DH plot, BJH plot, CI plot, INNES plot, MP plot, T-plot, etc, of PUS, assisted synthesized porous materials. In addition, BJH plot results confirm that the adsorbent particles prepared by ultrasound treatment are more uniform, finer and well-distributed. The application of PUS promotes the more distribution of adsorbent

particles; therefore, the performance of the adsorbent prepared with ultrasound treatment can be enhanced. The observed results indicate that the application of PUS in the method of preparation of adsorbent is an eco-friendly technique.

The present study beyond doubts proves that the application of PUS seems to be a potential alternative method for the preparation of adsorbent from agriculture waste materials. And also contribute to clarifying; standardize the presentation, nomenclature and methodology associated with the application of physisorption for surface area measurement and porosity analysis.

Keywords: PUS; ATR; FTIR; SEM; BET; XRD

OP-46

Removal of 'Pb' a Silent Killer in the Environment by an Adsorbent Derived from Litchi Chinensis

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Lead controversy in Maggi products is a hot subject of discussion during the past 3-4 years. As per the World Health Organization (WHO) standard the minimum permissible limit (MPL) of led have 0.1 ppm. Every day we come in contact with numerous substances natural or synthetic which are toxic. Lead is one such element that contaminates the environment and also enters the human body. Lead does not get destroyed even at high temperatures in the combustion chambers of automobile engines. It comes out as fine particles with the exhaust gases. The larger particle settles down soon, however, the finer ones remain suspended in the air depending upon the particle size and atmospheric conditions. Finally, the particles may settle down on various surfaces including soil, vegetation, buildings or on water bodies. An important source of lead in the lead-acid battery recycling facilities, Lead contamination of soil may also take place due to broken-down lead paint, discarded engine oil, pesticides used in agriculture, paint materials used in households and industries. Ageing lead paints can add high levels of lead to dust and soil. A very high percentage of Poly Vinyl chloride (PVC) pipes were found to contain lead. Source of lead in the pipes could be tin which is used as a stabilizer in the PVC pipes. Lead interferes with many enzymes which is an important reason for lead toxicity. It gets bound to sulfhydryl groups found in the enzymes in lieu of other metals like Ca, Fe and Zn that act as cofactors in the enzymatic reactions. One such enzyme is responsible for the synthesis of heme. That is why lead's interference also results in anemia. The WHO has accepted a new illness lead-caused mental retardation. In the case of acute poisoning abdominal pain, collapse, metallic taste, and paralysis may occur also gastrointestinal disturbance, undefined headache, peripheral neuropathy like foot and wrist drop takes place.

The objective of the present work is to evaluate the analytical potential of an adsorbent derived from agricultural waste Litchi Chinensis for effective removal of lead from its aqueous solutions/contaminated waste water streams. The new adsorbent was analyzed by FT-IR, UV-VIS, BET, SEM, X-RD techniques. Effect of various process parameters such as the amount of adsorbate and adsorbent, pH, ionic strength, the temperature on adsorption will be investigated.

Keywords: Pb Contamination Adsorption, Litchi Chinensis, FTIR, BET, XRD

OP-47

Enhancement in Biodegradability of Biodegradable Polymers by Incorporating Starch Granules Using Ultrasonic and Rheological Techniques

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Starch is one of the most inexpensive and most readily available of all natural polymers. There is a lot of use of polymers/plastics in different areas. An advance method, Ultrasonic velocity measurement is a very fruitful and resourceful technique that can be adopted for the study of liquids, liquid mixtures and also for Polymer solution mixtures. The biodegradable rates of blends can be controlled to a certain extent depending on the constitutions of blends, and the mechanical properties of blends are close to those of traditional plastics like polyethylene, polyvinyl alcohol, polylactides etc.

The degradation process through weight loss with time period was studied. All the changes were verified by FTIR, SEM and TEM characterization techniques. It concludes that the rate of biodegradation depends on polymer's structures and environmental conditions like temperatures, pressure, humidity etc. The reduction of their sensitivity to humidity makes these materials suitable for the production of biodegradable films & other items to make environment clean and safe.

OP-48

Plastic Polymers, its Scope and Effect on Environment: A Future Threat

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Plastics are inexpensive, lightweight, strong, durable, corrosion-resistant materials, with high thermal and electrical insulation properties. The diversity of polymers and the versatility of their properties are used to make a vast array of products that bring medical and technological advances, energy savings and numerous other societal benefits. These are, chemically speaking, long chains or large cross-linked structures most commonly made up of a framework of carbon atoms. Plastics are very stable and therefore stay in the environment a long time after they are discarded, especially if they are shielded from direct sunlight by being buried in landfills. This waste rots and decomposes, and also produces harmful gases (CO_2 and Methane) which are both greenhouse gases and contribute to global warming. Landfills also pollute the local environment, including the water and the soil. Plastics have become a vital asset for humanity. We need more research to introduce biodegradability, taking into account different applications and the need for infrastructure to deal with biodegradable plastics at the end of our life. Though extensive research and new technologies have led to invent of newer and safer plastics, but drawbacks and challenges of plastics have never been resolved and impact is on the rise.

Keywords: Environment, Plastics Age, Biodegradable Plastics, Global Warming, Virgin Plastics

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OP-49

Effect of Potassium and Phosphorus Fertilization on Green Herb Yield of Some Medicinal Plants of Himalaya Region (Uttarakhand) India

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Origanum vulgare (oregano) and *Thymus serpyllem* (wild thyme) is a member of the Lamiaceae family and is an indigenous aromatic and medicinal plant of Europe and Asia(Mediterranean region). At present, it is cultivated the mild, temperate climates of in North America, Europe, Asia, North Africa, and America in a large scale due to its economic importance. However, studies on agronomic factors such as application of potassium humate and irrigation intervals as well as nitrogen fertilization on yield and essential oils of oregano have not been investigated thoroughly until now. The observation on plant growth, yield per hectare, leaf area index, rhizome yield will be recorded. Profit would be examined and production will be popularized among local youth. it is commercially grown. The objective of this study was to examine the effects of different level of N, P and K on green herb yield and some herb chemical constituents (N, P, K) in order to recommend a reliable nutrient management for commercial growers. Results showed that, yield generally increase in accordance with the increases in N, P and K fertilizer rates.

Keywords: Nitrogen (N) Potassium (K), Phosphorus (P), Oregano (*Origanum vulgare*). Thyme (thymus serpyllem)

OP-50

Carbon Dioxide in High Value Product: Graphene

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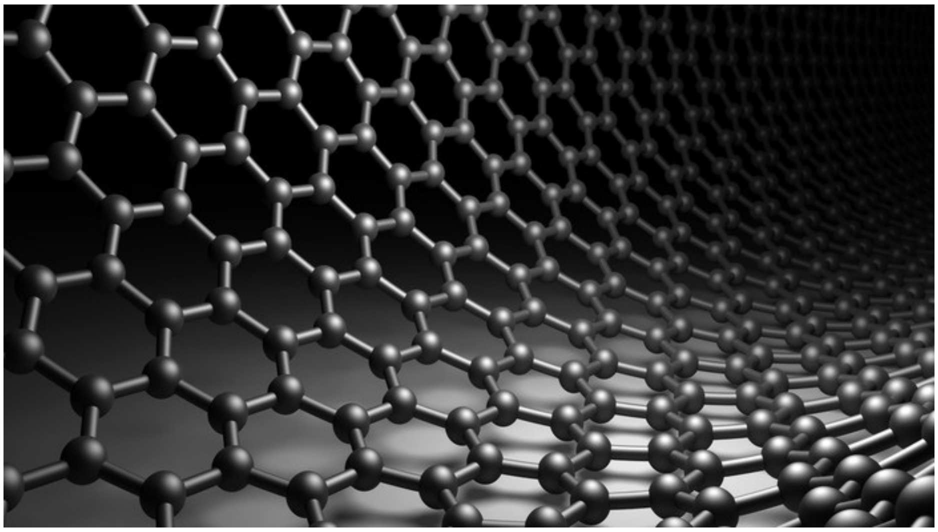
The green house gases water vapor, carbon dioxide, methane, nitrous oxide and ozone absorbs and emits radiant energy within the thermal infrared range coming from the vast majority of anthropogenic carbon dioxide emissions (i.e. emissions produced by human activities) come from combustion of fossil fuels, principally coal, oil, and natural gas resulting increase in earth temperature.



The major green house gase CO_2 can be converted into valubale nanosheets graphene, graphite and other high value products. Graphene may be synthesized using the chemical vapour deposition (CVD) method with the aid of a novel Ni–Ce–Fe trimetallic catalyst and also by a modular, cost effective "membrane contactor" that captures carbon dioxide (CO_2) from the exhaust gas sources and through a proprietary process.

OP-51

Sterically Hindered Rganobismuth Compounds Tris (α-Naphthyl) Bismuth(Iii) (α-C$_{10}$h$_7$)Bix$_{3-n}$(n=1,2) And Tris(α-Naphthyl)Bismuth (V) (α-C$_{10}$h$_7$) BiX$_{5-N}$ (n=2,3,4) Derivatives

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A voluminous amount of work on organometallic compounds of bismuth both in +3 and +5 oxidation has been reported in the past few years but the work is mainly confined to the derivatives based hydrocarbon residue like phenyl, methyl haloalkyl (-CF$_3$),halophenyl (-C$_6$F$_5$) etc. bonded to meta atom and only limited work has been reported on compounds having sterically hindered naphthyl, Cyclohexyl or mesityl groups. The introduction of the latter groups render hydrolytic and thermal stability compared to phenyl based analogues [1-20]. The nature and chemical behavior of bismuth compounds issomewhate different from antimony and arsenic. For example the oxidative reactions with electrophilic reagents like (SCN)$_2$ is preferred with triarylantimony and triarylarsenic compounds but in case of bismuth compounds cleavage of organic group is preferred over cleavage reaction.

$$A^{r}{}_{3}Sb + (SCN)_2 \longrightarrow A^{r}{}_{3}Sb(NCS)_2 \qquad \cdots\cdots\cdots(1)$$

$$A^{r}{}_{3}Bi + (SCN)_2 \longrightarrow A^{r}{}_{2}BiNCS + A^{r}SCN \qquad \cdots\cdots\cdots(2)$$

However in case of bulky groups stability of cyclohexyl or naphthyl group bonded to arsenic, antimony and bismuth compounds is more pronounced over the other organic derivatives of these metals.

A perusal of literature reveals that cyclohexyl and naphthyl based compounds of arsenic and antimony have been studied to a considerable extent but the information on organobismuth compounds is trivial. The synthesis of tris (α- naphthyl) bismuth was reported by challenger in 1914 [21] along with (α-naphthyl)$_3$BiCl$_2$ (α-naphthyl)$_2$BiCl and (α-naphthyl)$_3$BiBr$_2$. Since then some work on imides, amides and carboxylates has been done particularly by our research but the chemical behavior of (α- naphthyl)$_3$Biand its derivatives is yet to be studied

Thus the object of the present work was two fold (i) oxidative addition or cleavage reaction of tris(α- naphthyl) bismuth(III) employing halogens, pseudohologens and inter halogens and Metallic halides (ii) To examine the stability of naphthyl based derivatives of bismuth vis-à-vis phenyl derivatives along with their biological activity.

The paucity of the published data on sterically larger organobismuth compounds with α- naphthyl moieties encouraged us to undertake a systematic study on the

1. Synthesis and isolation of four different types of bismuth(III) halides and bismuth (V) halides having varying content of bulky α- naphthyl groups,R$_n$BiX$_{3-n}$,(α-C$_{10}$H$_7$)BiCl$_2$ reported earlier has also been obtained through redistribution reaction.

2. Synthesis and isolation of α- naphthyl bismuth (V) dichloride R_nSbCl_{5-n} (n=1,2) and mixed halides $RBiCl_2Br_2$.
3. Mixed halo carboxylates of the formula (α-$C_{10}H_7$)BiClL and (α-$C_{10}H_7$)BiLL'(L=monocarboxylates; L'=dicarboxylates) and (α-$C_{10}H_7$)BiL_2.
4. Synthesis of halo-imides of the type (α-$C_{10}H_7$)BiClL
5. Synthesis of halo oximates (α-$C_{10}H_7$)BiClL

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OP-52

Triphynylantimony(V) Carboxylates and Cycloantimonates; Biological Perspective, Screening & Assessment of Cyclotoxic, Antifungal and Antitumour Activity

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The synthesis and characterization of a number of triphynylantimony derivatives has been reported. In several cases structural conclusions have been derived with the aid of spectroscopic evidences and X-ray crystallogrophy. These studies were mainly involved to solve the problem of trigonal-bipyramidal (TBP) or square-pyramidal (SP) geometry which has been frequently established in case of phosphorus. The preferred geometry of Group 15 elements is a TBP which is fluxional, stereochemically non-rigid or pseudorotating arrangement rapidly interconverting with the alternative square-pyramidal structure. The energy different between the two structural alternative is small both in solution and in the solid state where the nature of the counterion for charged species lattice effects and the solvent of crystallization play a determining role. In this way, delicate balance exists between the TBP and SP forms, both in solution and the solid state. An appreciation of the pseudorotation processes occurring the life time of a five coordinate intermediate is clearly important for predicting and ultimately controlling product stereochemically.

The main concern of the investigation has been with the stereochemically of the pentavalent antimony derivatives and the biological aspects have seldom been looked into. Though in a number of cases organoantimony(V) derivatives along with organoantimony(III) derivatives have shown remarkable antimicrobial and antitumour activity.

The present investigation on organoantimony(V) carboxylates and cyclometallates was under taken with a view:

- To investigate chemical behavior as well as constitution of organoantimony(V) carboxylates, linear or polymeric and change in the nature of organoantimony(V) carboxylates on changing the carboxylic group.
- To isolate hitherto unreported organoantimony(V) carboxylates.
- To investigate the biocidal and antitumour activity associates with organoantimony(V) -carboxylates and -cyclometallates.

Since one of the major aims of presents investigation was focused on the biological activity of organoantimony compounds, the author synthesized a series of triphenylantimony(V) derivatives with salicylic acid, benzillic acid, mandelic acid and its derivatives, aspartic acid, 2-pyrazine carboxylic acid and naproxene. The structure of few compounds is well established by X-ray differaction method and therefore in turn helped to established structure activity relationship

OP-53

Studies on Pentafluorophenyl Arsenic (III) Corboxylates

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Despite a considerable interest in the chemistry of hydrocarbon based organoarsenic(III)corboxylates of the general formoula R_2AsL and $RAsL_2$, those containing pentahalophenyl group (s) C_6F_5 and C_6Cl_5 have not been studied so for In sharp contrast to this taking cue from the fact that arsenic containing organometallic compounds both in +3 and +5 oxidation state exhibit antitumor,antifungal and antibacterial activity. we now intrest this synthesis of pentafluorophenyl based derevatives of arsenic(III) particularly carboxylate derevatives expected to be biologically active.

It may be noted that fluorine based compounds are water and lipid soluble enhancing their biological activity coupled with corboxylate moiety are further expected to exhibit investigation thus respect the synthesis structure and biological activity of its compounds of the type $(C_6F_5)_2AsL$ and $(C_6F_5)AsL_2$.where L is a corboxylate moiety .the newly synthesis compounds have been identified on the basis of spectrochemical evidence.DFT calculation have been useful in establishing structure reactivity relationship added by experimental results.

Keywords: Pentafluorophenylarsenic (III)Corboxylates Synthesis, Spectroscopy, DFT Calculations Activity

OP-54

Pomegranate Juice Protects Nitric Oxide Against Antioxidant Destruction and Enhances the Rejuvenation

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Pomegranate juice (PJ), which is a rich source of potent flavonoid antioxidants, was tested for its capacity to protect nitric oxide (NO) against oxidative destruction and enhance the biological actions of NO. Employing chemiluminescence head space analysis, PJ was found to be a potent inhibitor of superoxide anion-mediated disappearance of NO. PJ was much more potent than Concord grape juice, blueberry juice, red wine, ascorbic acid, and DL-a-tocopherol. As little as 3 μl of a 6-fold dilution of PJ, in a reaction volume of 5000 μl, produced a marked antioxidant effect, whereas 300 μl of undiluted blueberry juice or nearly 1000 μl of undiluted Concord grape juice were required to produce similar effects. PJ and other antioxidant-containing products were found to augment the anti-proliferative action of NO (DETA/NO) on vascular smooth muscle cell (rat aorta) proliferation. PJ was much more effective than the other products tested and elicited no effects when tested alone in the absence of added NO. Similarly, neither PJ nor the other products enhanced the anti-proliferative action of a-difluoro methylornithine, a stable substance that inhibits cell growth by NO-independent mechanisms. In order to determine whether PJ is capable of increasing the production of NO by vascular endothelial cells, PJ was tested for its capacity to up regulate and/or activate endothelial NO synthase (eNOS) in bovine pulmonary artery endothelial cells. PJ elicited no effects on eNOS protein expression or catalytic activity. Moreover, PJ did not enhance promoter activity in the eNOS gene (COS-7 cells transfected with eNOS). These observations indicate that PJ possesses potent antioxidant activity that results in marked protection of NO against oxidative destruction, thereby resulting in augmentation of the rejuvenation of NO.

Keywords: Nitric Oxide; Antioxidant Activity; Polyphenols; Flavonoids; Vascular Smooth Muscle Proliferation

OP-55

Synthesis of Biologically Active Natural Product Diptoindonesin G

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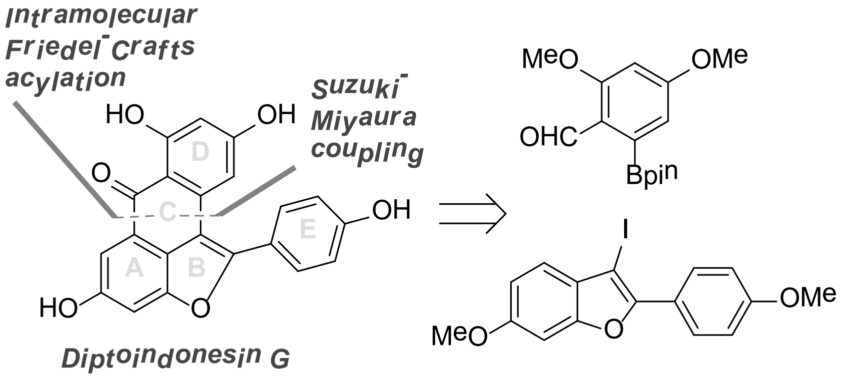

Diptoindonesin G, a tetracyclic oligostilbenoid natural product was first isolated from the tree bark of *Hopea mengarawan* in 2009. A convergent and scalable synthetic route to this tetracyclic oligostilbenoid natural product is described where Suzuki-Miyaura cross-coupling and intramolecular Friedel-Crafts acylation were employed to construct the central C ring of diptoindonesin G. Two fragments for cross-coupling reaction were readily synthesized with similar efficiency.

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OP-56

Characterization of Activated Bagasse Fly Ash (ABFA) For Sugar Decolorization

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ABSTRACT—Bagasse fly ash (BFA), a waste material generated in the sugar industry, collected from a local sugar factory, was used as a low cost and effective adsorbing surface for the removal of colourants from aqueous sugar solution. The raw material employed for the production of the new adsorbent is widely available across the world free of cost. The Physical (bulk density, hardness) and chemical properties (pH, conductivity, ash) of the activated BFA samples were analyzed using standard methods. Batch studies were performed to evaluate the adsorption capacity was followed as a function of pH, adsorbent dose, effect of ionic strength, shaking time, concentration of adsorbate and temperature. Under the optimum conditions used, more than 90% of the colourants under study were successfully removed. Relative efficiency of decolorization was compared with the commercial activated carbon (Darco Carbon) and ion exchange resin. It was found that the BFA showed the satisfactory physical and chemical properties. The decolorizing property was much better than the commercial carbon making it a good decolourizer in the sugar refinery/industry.

POSTER PRESENTATION (PP)

PP-01

Synthesis and Characterization (bis-benzyl) Tellurium Diiodide at Room Temperature

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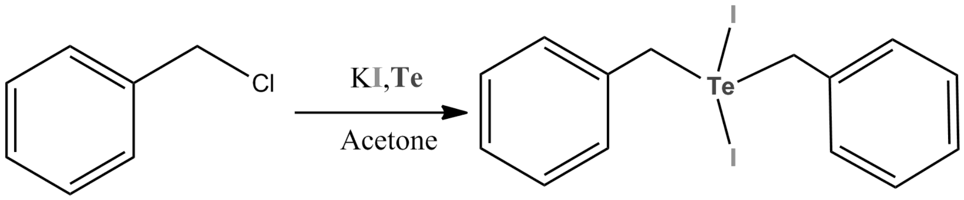
We are reported here the synthesis and characterization of bis-benzytelluriumdioiodide by the insertion of tellurium across carbon-halogen bond at room temperature. First we treated benzylchloride with tellurium metal after 24 hr reaction was unsuccessful. After this we added potassium Iodide within 30 minutes reaction mixture indicated the insertion of Tellurium across C-halogen bond takes place.



PP-02

Synthesis and Characterization CNN-Pincer Ligand

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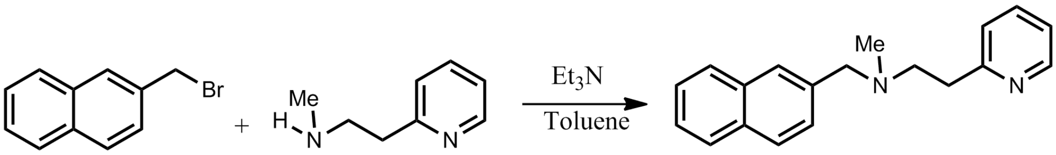
Preparation of novel unsymmetrical, tridentate ligand precursor, N-methyl-N-(naphthalen-2-ylmethyl)-2-(pyridin-2-yl) ethanamine has been described. To a solution of *N*-methyl-2-(pyridin-2-yl)ethanamine (2.80

ml, 20.0 mmol) and NEt_3 (10 ml) in freshly distilled dry toluene (50 ml) was added dropwise a solution of 2-(bromomethyl)naphthalene (4.40 g, 20.0 mmol) in same solvent (50 ml). After 1 h the resulting white suspension ($HNEt_3$-Br) was filtered and washed with dry toluene (25 mL). The filtrate was concentrated by removing the solvent in vacuum. This resulted in a light yellow semi solid residue, which was purified by Colum chromatography to yield as colorless oil (4.12 g, 74%). ES-MS m/z (relative intensity, nature of peak) 277 (100, $[MH]^+$). ^1H NMR (500 MHz, $CDCl_3$, 25 °C): *d* 2.30 (s, 3H, CH_3), 2.86 (t, 2H, CH_2), 3.01 (t, 2H, CH_2), 3.70 (s, 2H, CH_2), 7.04-7.14 (m, 2H), 7.38-7.45 (m, 3H), 7.50-7.58 (m, 1H), 7.66 (s, 1H), 7.72-7.80 (m 3H), 8.46-8.49 (d, 1H).^{13}C NMR (500 MHz, $CDCl_3$, 25 °C):*d* 36.0, 42.1, 57.3, 62.3, 121.1, 123.2, 125.5, 125.9, 127.3, 127.5, 127.6, 127.7, 128.0, 132.8, 133.3, 136.2, 149.2, 160.3.



PP-03

Reinvestigation of Synthesis of Silver Nanoparticle using Guava (Pisidium Guajaja) Leaf Extract

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Among the various inorganic nanoparticles Silver nanoparticles have received substantial attention in the field of Green Synthesis. The extensive use of Silver Nanoparticles needs a synthesis process that is greener without compromising their properties. The present synthesis describe a novel green synthesis of Silver Nanoparticles using Guava leaf extract ,which prepared by soaking and boiling of chopped guava leaf with deionized water and used as reducing agent . Fourier Transform Infrared Spectroscopic analysis of the used extract and as synthesized silver nanoparticles suggests the possible reduction of Ag+ by the water soluble ingredients of guava leaf like Tannin, Eugenol and flavonoid .in this synthesis reaction of leaf extract of guava and Silver Nitrate(AgNO3) solution occurs . The green synthesized Silver-Nanoparticles are characterized by UV-Visible and TEM analysis.

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PP-04

Quantum Chemical Designing of 10, 11 -dihydro-5H-dibenz [b,f] Azepine Dyes with D-π-A Configuration for Dye Sensitized Solar Cells and Studying the Effect of Acceptor on Performance of DSSCs

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Three new 10,11-Dihydro-5H-dibenz [b,f]azepine based dyes were designed, utilizing different acceptor groups and understand their roles in dye-sensitized solar cells (DSSCs). The computational techniques are used to study the effect of acceptor in π-conjugated systems on absorption spectra and electron injection of the dyes. Three dyes were studied ie. (E)-3-(4-(10,11-Dihydro-5H-dibenz[b,f]azepine) oxazol-2-yl)-2-cyanoacrylic acid (**Dye 1**), (E)-3-(4-(10,11-Dihydro-5H-dibenz[b,f]azepine) oxazol-2-yl) vinyl)pyridin-1(2H)-yl) acetic acid (**Dye 2)**, (E)-3-(4-(10,11-Dihydro-5H-dibenz[b,f]azepine)oxazol-2-yl)methylene)-4-oxo-2-thioxothiazolidine-3-carboxylic acid (**Dye 3**) with 2-cyanoacrylic acid, pyridin-1(2H)-yl) acetic acid, Methylene-4-oxo-2-thioxothiazolidine-3-carboxylic acid**(Rhodanine-3-acetic acid) as the acceptor in DSSCs**. In theoretical examination Optical and electronic properties, UV–Vis absorption spectra ,light harvesting efficiency (LHE) have been calculated. All the calculations were done DFT calculation at B3LYP by using 6-31+ G** to evaluate the effects of various acceptor group on the optical and electronic properties of the dyes in dye-sensitised solar cells. Optical properties were calculated using the time-dependent DFT calculations with the B3LYP and CAM-B3LYP.

Keywords: DSSCs, Optical Properties, LHE, DFT Method

PP-05

Electrical Conductance Studies for Parchment Supported Iron Tungstate Model Membrane

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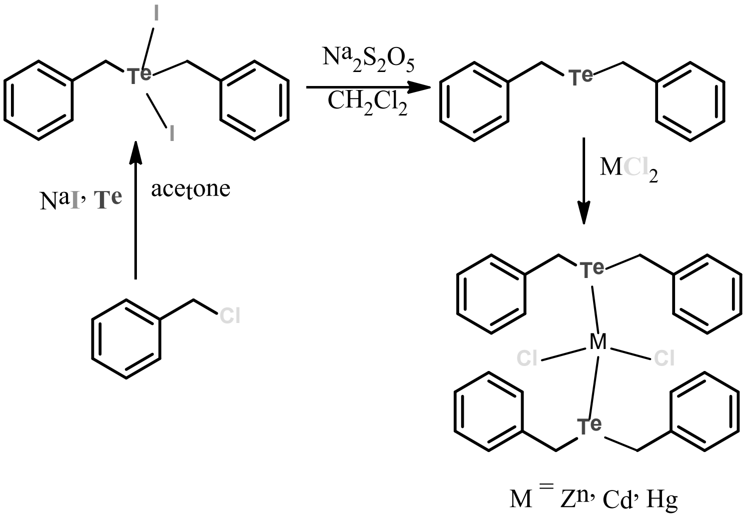
Electrical conductance of parchment supported model membrane bathed in different concentration of 1:1 electrolytes (KNO_3, $NaNO_3$ and NH_4NO_3) at several temperature ranges are reported. An increase in

conductance with increase in temperature may be due to the state of hydration. The model membrane have been characterized on the basic of TGA, DSC, TEM, SEM, FTIR and XRD analysis.



PP-06

Etherification of Glycerol with *tert*-Butyl Alcohol: For Future Biodiesel

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Herein we reported that the etherification of glycerol with *tert*-butanolin the presence of sulphonated -silica, -cellulose, MIL-101(Cr), acid resin and amberlyst-15 as catalyst. The effect of reaction conditions and conditions for optimal selectivity towards etherification is investigated. The maximum conversion of glycerol (~95%) is obtained at 80 °C and at the molar ratio *tert*-butanol/glycerol (4) after 5 hr. In two step reaction selectivity towards poly-ethers was close to 58% with a simplest reaction setup in 10 h. An easiest protocol to separate mono-*tert*-butyl glyceryl ether and di-*tert*-butyl glyceryl ether from reaction mixture is also proposed. These separated samples are used as reference sample in Gas Chromatogram analysis. The Catalytic activity of sulphonated-silica is compared with sulphonated MIL-101(Cr), cellulose, acid resin and Amberlyst-15 resin. A plausible mechanism for etherification of glycerol and reverse reaction of mono-*tert*-butyl glyceryl ether into glycerol and *iso*-butene is reported.

PP-07

Review on Synthesis and Applications of Copper Nanoparticles via Biogenic Process

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The interest on copper nanoparticles and their synthesis have been increased over past few decades. This has resulted in the generation of copper nanoparticles by chemical and physical methods. Because of use of different toxic chemicals and solvents, these methods are not so fruitful for the synthesis of different shaped and sized copper nanoparticles. So an alternate method for the synthesis of copper nanoparticles has been used. These methods use different living organisms such as fungi, bacteria and plants. These methods have many properties such as green method, eco and environmental friendly and there is no use of different toxic chemicals and the equipment's used in these greener methods of synthesis of copper nanoparticles. This paper gives an overview on the ecofriendly and biological synthesis and about the uses of different copper nanoparticles. It also highlights the importance and positive and negative impact on human as well as on environment.

Keywords: Green Synthesis, Biogenic Process, Copper Nanoparticles

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PP-08

Synthesis, Spectral Analysis, DFT Calculations of Zn(II) Coordination Compounds with Schiff Bases Derived from S-benzyldithiocarbazate

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Novel Zn(II) complexes of benzyldithiocarbazate has been synthesized and characterized by elemental analysis, IR, Raman, EI-MS, UV–Vis, ^{1}H NMR, ^{13}C NMR and TGA analysis. IR spectra reveled that the ligands were coordinated to the Zn(II) in a bidentate form with NS donor sites.. The dithiocarbazate Schiff bases coordinate as a uninegatively bidentate NS chelating ligands via the azomethine nitrogen and the thiolate sulfur atoms. DFT and TD-DFT calculations on the complex were also carried out by the B3LYP/6-311++G(d,p)/ LanL2DZ basis set levels of theory. The results were used to molecular orbital diagram, HOMO–LUMO, NBO, spin-

allowed singlet-singlet electronic transitions studies (TD-DFT) and electrostatic potential were in conformity with calculated results. VEDA 4 (Vibrational energy distribution analysis) software was employed for theoretical FT-IR spectrum analysis for fundamental vibrational modes along with potential energy distribution percentage (PED%) showing non-linearity of [Zn(L)$_2$] complexes.

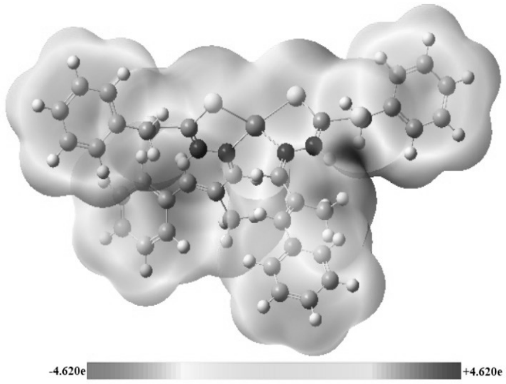

Fig. 1: 3D Plots of MEP of [Zn^{II}(sbalm)$_2$]

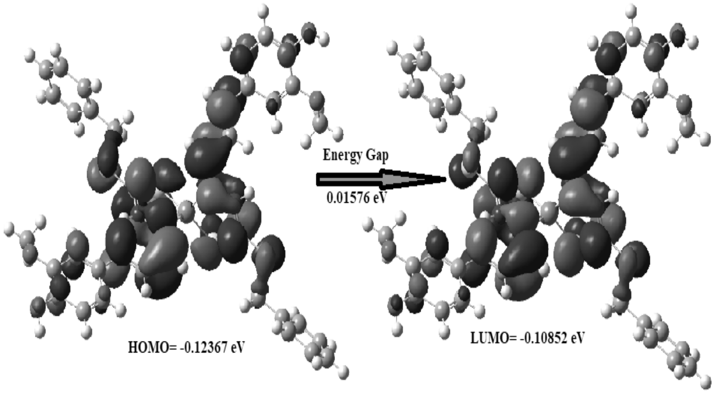

Fig. 2: 3D Plots of Frontier Molecular Orbitals of [Zn^{II}(sbcin)$_2$]

PP-09

Comparative Haematological Studies using Pituitary Gland Extract and Ovaprim in Cyprinus Carpio

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Haematological parameters used as diagnostics tools to assess the health status of fish and these parameters varied according to season, sex, and hormonal change. The purpose of the present study was to know the effect of ovaprim and pituitary gland extract hormone injection in Cyprinus carpio by analysis of some parameters such as RBC, WBC, Hb, PCV, MCV, MCH, MCHC and blood glucose of the experimental fish and compared in relation to sex and pre and post spawning after hormonal injection. The brooders (male & female) were treated separately with ovaprim and PGE. The results show higher value of RBC, Hb, PCV, MCH, and MCHC in male before hormonal injection. After treatment RBC, PCV, Hb, MCV, MCH, MCHC were decreased, while glucose increased. The male & female brooders treated with ovaprim have higher value of WBC and glucose compare to PGE.

PP-10

Ozone Layer Depletion

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The stratospheric ozone layer forms thin shield in the upper atmosphere which protects the life from harmful ultraviolet (UV) rays. Several studies found evidences that the ozone layer is being depleting. Depletion of ozone layer results in increased UV radiation reaching the earth surface which in turn greater exposure of UV radiation at the surface effects environment. In this paper we present that ozone layer depletion occurs through catalytic chemistry involving man-made chlorofluorocarbon is the area of study in global issues. Now a days various anthropogenic activities such as emission of CFCs, HCFCs and others organ halogens leads to deplete ozone layer. The chemical reaction mechanism operating with the ozone layer has been also including very efficient the chemical species, (NO, $NO_{2,}$ Cl, ClO). Some evidences come from direct measurement of increasing ozone depleting substances by using man-made chemicals. There are many efforts like Clean Air Act, Montreal Protocol and prevention of ozone is done for protecting the ozone layer. This paper deals a brief history of ozone depletion & conceptual framework to explain key process involved.

Keywords: Ozone, Ultraviolet Rays, Stratosphere, Chlorofluorocarbons (CFCs)

PP-11

A Review on Green Synthesis of Palladium Nanoparticles

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Nanomaterial synthesis is an enormously growing field of science and researchers have shown a great interest in the synthesis of metallic nanoparticles using different methods. Pd NPs have a wide range of applications in different areas, for example as catalysts for various chemical transformations, carbon-carbon bond formation, fuel cell electrochemical reactions, hydrogenation reactions, cross-coupling reactions and so on. Therefore, developing green methods for the synthesis of Pd NPs is of highly desirable. We have focused on biogenic synthesis of Pd nanoparticles such as plant extract, micro-organism, algae and biodegradable polymers. Natural products such as polyols, polyphenols, flavonoids, proteins are the major reducing and stabilizing agents in synthesis of Pd NPs. The foremost purpose of the present contribution is to highlight the most reliable, cost-effective and environment-friendly synthetic protocols for preparation of Pd NPs of different size, shape, composition, and with a high degree of monodispersity. In this work, we have given an outline the available data of green synthesis of Pd NPs till now.

Keywords: Green Synthesis, Biogenic Synthesis, Palladium Nanoparticles

PP-12

Synthesis and Characterisation of Chromium(ш) Compound with Tetra Dentate S_4 Macrocyclic Ligands

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The chemistry of macrocyclic ligands and their complexes has varied applications in the area viz. medicinal, biochemical, environmental, industrial, photochemical, photophysical, photoelectronic etc.Synthesis of the complexes- The reaction is carried out in 1:1 molar ratio 0.9-0.8 gm ligands $MacL^1$-$MacL^{44}$ were dissolved in methanol. The reaction is followed by the addition of $CrCl_3.xH_2O$ and $Cr(NO_3)_2.xH_2O$ The resulting mixture was stirred for 12 hours at 0°C, the solid product was obtained by filtration and washed repeatedly with same solvent and dried in vacuo. The product were recrystallized from benzene.

PP-13

Pollution Prevention: Fundamental Analysis and Review of Latest Researches

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For the sake of healthy living of our upcoming generations, it is important to have a sustainable environment which is not harmful to living beings. Currently, the problem of environmental pollution is a big concern regarding this. In the written research article, fundamental analysis of environmental pollution has been done by reviewing the recent concepts recognized through latest research papers and other publications. After that, the status of environmental pollution has been analyzed through recently done research works as well as by obtaining some other standard data. Then some solutions have been suggested based upon the research results those have been confronted.

Environmental Pollution is basically contamination of physical, chemical and biological components of our environment. Unhealthy change in temperature, pH levels, basicity or acidity is said to be physical contamination, whereas chemical contamination means the introduction of chemical pollutants to the environment and biological contamination means such a change in the environment which makes harmful microbes habitable in our environment. For having the idea of the hazardous level of pollution the notable fact here is the world's 91% of the population is living in the places exceeding the World Health Organization's prescribed guidelines. Air pollution kills more than 1 million people in India per year. The greenhouse gases are destroying our environment to such an extent that it is being unrecoverable. That is why control over the emission of greenhouse gases is very much needed and recent research works ignite the hope for the same.

For the purpose of converting greenhouse gases to valuable materials, the work is being done at the global level by many institutions. Such a work is the work being continued in Linkoping University, Sweden where the researchers are working on converting CO2, and water to a renewable energy source [based on the concept that essential energy fuels have the same structural elements as in them (C, H & O)]. Artificial photosynthesis is also noteworthy. All the above-mentioned works and some others have been deeply analyzed in the full research article.

Keywords: Environment, Greenhouse Gases, Pollution Prevention, Renewable Energy

PP-14

Green Synthesis of Silver Nanoparticles and its Various Applications: A Review

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Since recent years, the global survey evidenced the scope of nanomaterials and nanotechnology in the field of medicine and their radioimmunoassay techniques. Due to their **nontargeted specificity**, a number of nano's has been prepared, doped with an enzymes surfactant to act on specific targetting cells like MCF-7 breast cancer and A-549 lung cancer. Current studies show that green synthesis of nanoparticles is one of the most emerging field of nanotechnology, Metallic nanoparticles have been widely used for biomedical application and among them, silver nanoparticles (Ag NPs) are highly remarkable due to its unique properties, such as catalytic activity, antimicrobial activity, pharmaceutical, biosensors, and photothermal therapy. Green synthesis of Silver Nanoparticles using plant extract, bacteria, fungi, yeast, actinomycetes have a new scope of research for scientists and researchers. Biogenic synthesis of Ag NPs can extremely reduce the pollution rate and also decreasing the risk to human health as the consequences of using toxic chemicals and solvents in global air samples and contaminated soil. The material used for biogenic reduction of silver salt is easily available in our environment, cost-effective and eco-friendly. Natural compounds such as proteins, enzymes, alkaloids, flavonoids, steroids, tannins, and other nutritional compounds act as reducing, stabilizing and capping agent and have been used for the synthesis of silver nanoparticles. These natural compounds are extracted from different parts of the plant. In this review, we have tried to summarize the available literature of green synthesis of silver nanoparticles so far.

Keywords: Green Synthesis, Silver Nanoparticles, Catalytic Activity, Antimicrobial Activity, Biogenic

PP-15

Exploring Blood Parameters and Interleukins IL-17F and IL-17A Levels for Asthma Diagnostics

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Introduction: Asthma is a multi-factorial disorder and both genetic and environmental factors contribute to its development. The lack of diagnostic tools and biomarkers for the early detection of asthma limits the early therapy and management of the disease.

Aim: We have, therefore, investigated the levels of some serum parameters that may be used for early diagnostics in asthma.

Methods: 100 elderly asthmatics and equal number of healthy elderly individuals were selected for this study. Asthmatic patients were confirmed by Spirometry (lung function test), IgE level and examination of other clinical parameters. Serum total IgE levels,IL-17A and IL-17F levels were measured by ELISA and compared to the healthy controls and relative quantification was determined and correlated in a case control study.

Result: We observed that asthmatics of same height and age had lower weight and higher smoking rate in comparison to controls. The other parameters namely, breathlessness, cough, headache, disturbed sleep, congestion, and wheezing were recorded to be significantly elevated in asthmatics than in controls. Excepting Hb, levels of blood eosinophils, Acute Eosinophilic Count, T-Lymphocyte Cells and serum IgE were higher in asthmatics than in controls. The lower serum IL-17F and IL-17A levels recorded in asthmatics have positive correlations with levels of IgE. These interleukins were also found to have positive correlation among each other.

Conclusion: These observations and results from clinical diagnostic symptoms and biochemical analysis reflect that the blood parameters monitored in the study may serve as potential markers for early detection of asthma. These parameters may be implicated in the early detection, diagnosis and adequate management of the disease.

PP-16

Zinc Oxide and Titanium Dioxide Nanoparticles Application in Biosensor: A Comparative Study

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[2]Government Science College Gwalior

Development of nanomaterial and their application for cancer detection with the help of biosensor is a centre of scientific attention in recent years. Here we are reporting Highly Effective and economic zinc oxide and

Titanium dioxide biosensors for the detection of carcinogenic gases. It has been found by the health and safety executive that workers exposed to 1 microgram per metre cube for a period of 40 years are 8% more likely to develop lung cancer, tobacco, Char grilled meat also causes Cancer, so diagnosis of early cancer is highly demanding .

This work was done in successive steps first, growth of nanomaterial thin films on glass surface and its characterisation, second study of grown nanomaterials thin films exposed to carcinogenic gases.

Thus one of the important field where the advancement is crucial a new Diagnostic technique is required. We concluded that Zinc oxide, Titanium dioxide, potentials in biosensing field can be used as human cancer biomarker detection.

PP-17

Green Synthesis of Carbon Nanoparticles (Cnps) from 2-Acetoxybenzoic Acid (Disprin): Synthesis, Characterization and Preliminary Study of Cultivation of Fluorescent Flowers

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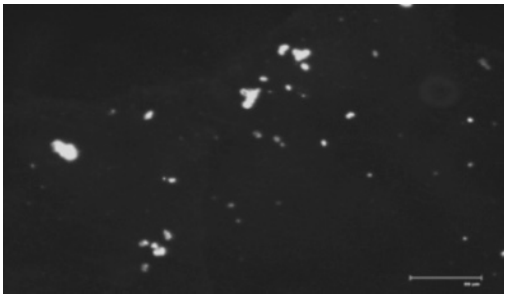
Strongly fluorescent carbon nanoparticles (CNPs) were simply prepared by microwave-assisted synthesis using 2-Acetoxybenzoic acid, a non-steroidal anti-inflammatory drug (NSAID).. The aqueous solution of Disprin, with a concentration of 1 g per 10mL, was exposed to microwave radiations for a total period of 2 min. The carbon nanoparticles, [1-2] as synthesized, were characterized by various analytical techniques such as Fourier Transformation Infra-Red (FTIR) spectroscopy, X-ray diffraction(XRD), Transmission Electron Microscopic (TEM) analysis, UV-Vis spectroscopy, and Fluorescent Microscopy(FM) etc. The XRD pattern indicated presence of a few characteristic peaks, obtained from reflections through various planes. SEM and TEM analysis confirmed the size of the CDs, which had a narrow size range of 20 to 60 nm. The CDs, thus produced, showed a strong fluorescence when exposed to UV radiations. The UV spectrum of as synthesized carbon dots showed a strong absorption at around 260 nm. The TEM analysis revealed that 40 % of the particles had diameter in the range of 20 to 30 nm, while 15 % had their size less than 10 nm. Zeta potential was found to be -3.65 mV, thus indicating presence of slight negatively charged surface. Finally, the highly photoluminescent CDs obtained were used to cultivate fluorescent carnations by a water culture method, While the results of fluorescence microscopy analysis indicated that the CNPs had entered the plant tissue structure. It was observed that the carbon nanoparticles were used to image in the cells and fluorescence imaging will be performed. It was observed that the flowers, cultivated in CDs containing water showed a brilliant fluorescence while the other flower, cultivated in distilled water did not show any sign of fluorescence.



CNPs Showing Green Fluorescence

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PP-18

Carbene-Catalyzed Redox Alkenylation of Isatins using β-Substituted Organo-Selenones and Aldehydes

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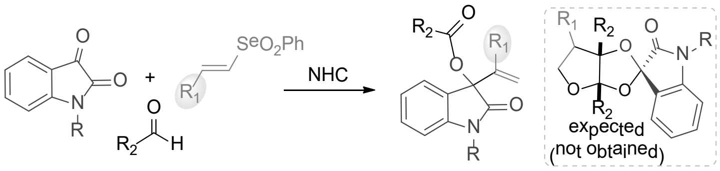

The catalytic fusion of several components in one-step, generating a highly functionalized moiety, offers an alternate and a greatly sought strategy in organic synthesis over the conventional multi-step synthesis due to its inherent efficiency, atom-economy and molecular diversity. On the other hand, C-3 functionalized oxindoles are omni-present in numerous biologically active molecules and drug candidates. Accordingly, the direct manipulation of carbonyl functionality in isatins through Multi Component Reactions (MCRs) has recently attracted huge attention. Achieving several desired transformations in a single operation remains one of the obvious goals in the synthetic organic chemistry.

Here in, we have developed a MCR for the direct alkenylation of isatins through the NHC-catalyzed redox reaction in the presence of β-substituted vinyl selenones and aldehydes. The challenging β-substituted vinyl selenones reacted smoothly under the NHC-catalysis to give the various products, which are otherwise challenging to prepare using literature known methods. The products are advantageously obtained as esters (a protected quaternary alcohol) in a single operation, thereby, eliminating the undesired protection step for further transformations.

PP-19

Environmentally Benign Mechanistic Studies of the Oxidation of Glucose in Alkaline Medium: A Kinetic Approach

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Almost everyone enjoys sugars and sweets, but many consumers wonder whether consumption of sugars affects health. Carbohydrates are vital to human survival and it somewhat surprising that their study took so long to emerge as a glamorous area of research. Carbohydrates are present in nucleic acids and are thus vital in controlling proteins synthesis and in transmission of genetic information with other. In pharmaceutical industry; glucose is used as a precursor to make vitamin C (L-ascorbic acid) in the Reichstein process, to make citric acid, gluconic acid, polylactic acid and sorbitol. The mammalian brain depends on glucose as its main source of energy. In the adult brain, neurons have the highest energy demand, requiring continuous delivery of glucose from blood. Glucose is used to treat very low blood sugar (hypoglycemia). Most often in people with diabetes mellitus .Glucose is given by injection to treat insulin shock and it works by quickly increasing the amount of glucose in our body. Due to this reason I have been investigated the Ir(III) – catalysis of the iodate oxidation of glucose in aqueous acidic medium oxidation of glucose in alkaline medium. The reaction exhibits first – order kinetics with respect to lower IO_3 and [OH] and show zero order kinetics at their higher concentration where as zero order kinetics with respect to [glucose] was observed throughout its variation. The reaction shows first order kinetics with respect to Ir (III) in the oxidation of glucose.

Keywords: Carbohydrates, Glucose, Potassium Iodate, Iridium Catalyst, Sodium Hydroxide, Kinetics

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PP-20

Global Warming

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Global warming is the term used to describe a gradual increase in the average temperature of the Earth's atmosphere and its oceans, a change that is believed to be permanently changing the Earth's climate. There is great debate among many people, and sometimes in the news, on whether global warming is real (some call it a hoax). But climate scientists looking at the data and facts agree the planet is warming. While many view the effects of global warming to be more substantial and more rapidly occurring than others do, the scientific consensus on climatic changes related to global warming is that the average temperature of the Earth has risen between 0.4 and 0.8 °C over the past 100 years. The increased volumes of carbon dioxide and other greenhouse gases released by the burning of fossil fuels, land clearing, agriculture, and other human activities, are believed to be the primary sources of the global warming that has occurred over the past 50 years. Scientists from the Intergovernmental Panel on Climate carrying out global warming research have recently predicted that

average global temperatures could increase between 1.4 and 5.8 °C by the year 2100. Changes resulting from global warming may include rising sea levels due to the melting of the polar ice caps, as well as an increase in occurrence and severity of storms and other severe weather events. The presence of radiatively active gases in the Earth's atmosphere (water vapour carbon dioxide, and ozone) raises its global mean surface temperature by 30 K, making our planet habitable by life. There has been an increase in carbon dioxide and other trace gases since the Industrial Revolution, largely as a result of man's activities, increasing the radiative heating of the troposphere and surface by about 2 W m−2. This heating is likely to be enhanced by resulting changes in water vapour, snow and sea ice, and cloud. The associated equilibrium temperature rise is estimated to be between 1 and 2 K, there being uncertainties in the strength of climate feedbacks, particularly those due to cloud. The large thermal inertia of the oceans will slow the rate of warming, so that the expected temperature rise will be smaller than the equilibrium rise. This increases the uncertainty in the expected warming to date, with estimates ranging from less than 0.5 K to over 1 K. The observed increase of 0.5 K since 1900 is consistent with the lower range of these estimates, but the variability in the observed record is such that one cannot necessarily conclude that the observed temperature change is due to increases in trace gases. The prediction of changes in temperature over the next 50 years depends on assumptions concerning future changes in trace gas concentrations, the sensitivity of climate, and the effective thermal inertia of the oceans. On the basis of our current understanding a further warming of at least 1 K seems likely. Numerical models of climate indicate that the changes will not be uniform, nor will they be confined to temperature. The simulated warming is largest in high latitudes in winter and smallest over sea ice in summer, with little seasonal variation in the tropics. Annual mean precipitation and runoff increase in high latitudes, and most simulations indicate a drier land surface in northern mid-latitudes in summer. The agreement between different models is much better for temperature than for changes in the hydrological cycle. Priorities for future research include developing an improved representation of cloud in numerical models, obtaining a better understanding of vertical mixing in the deep ocean, and determining the inherent variability of the ocean-atmosphere system. Progress in these areas should enable detection of a man-made "greenhouse" warming within the next two decades.

PP-21

Construction of Phenanthrenes Via Facile Aryne Diels-Alder Reaction with B-Bromostyrenes as 4π-Components

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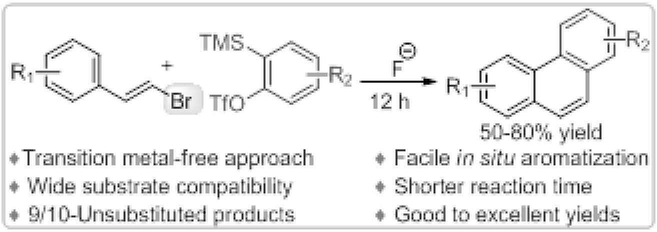

Phenanthrenes has received significant attention among the various polycyclic aromatic rings because of their presence in natural products and pharmaceutics like antiviral, anticancer and antimalarial agents along with huge applications in material chemistry due to their photochemical and electroluminescent properties.

Therefore a mild, selective and transition-metal free protocol for the synthesis of polycyclic aromatic hydrocarbons, predominantly phenanthrenes, is a highly desirable and challenging endeavor in organic synthesis. The transition-metal catalyzed methods has a very rich contribution to literature pool but still there is a need for a more effective transition-metal-free, environmentally benign, inexpensive and selective protocol for phenanthrene synthesis.

Herein, we have established a highly efficient transition metal-free method for the synthesis of phenanthrenes from β-bromostyrenes and arynes. The reactions proceed via Aryne Diels-Alder (ADA) reactions with β-bromostyrenes, followed by a facile aromatization. This protocol successfully circumvents the requirement of a strong electron-withdrawing group at the β-position of the styrenes which severely limits the scope of the method to only 9/10-substituted analogs. All the products were obtained in high yield without the formation of undesired side product. Mild and in-situ generation of arynes renders this methodology to tolerate wide functionalities. This method gains importance with easy availability of raw materials, efficient reaction, step/atom economy, mild reaction conditions, better yields and a broad scope.

PP-22

A Highly Efficient NHC-Catalyzed Aerobic Oxidation of Aldehydes to Carboxylic Acids

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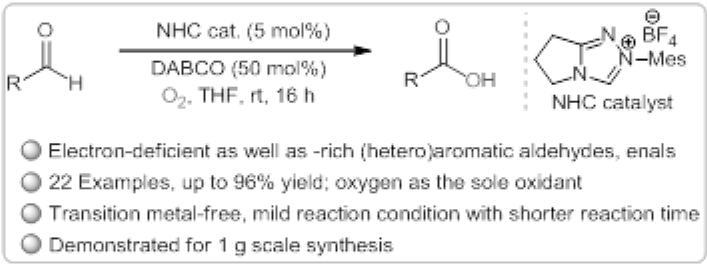

- Electron-deficient as well as -rich (hetero)aromatic aldehydes, enals
- 22 Examples, up to 96% yield; oxygen as the sole oxidant
- Transition metal-free, mild reaction condition with shorter reaction time
- Demonstrated for 1 g scale synthesis

Carboxylic acids are one of the most encountered functionalities in organic compounds used in pharmaceuticals, agrochemicals and industrial chemicals. In general, this class of compound is prepared via oxidation of the corresponding alcohol or aldehyde. Therefore, the oxidation of aldehydes to their carboxylic acid counterparts is a fundamentally significant organic manipulation with a huge industrial application. Numerous metal-based oxidants have been developed, e. g., chromates, permanganates, perchlorates, peroxides, etc. Metal-free organocatalysis has been extensively explored as the alternate mode of activation for a variety of transformations earlier known to be catalyzed only by a metal-complex. This distinctly offers several advantages over metal-based approach like robust in operation, availability, greener and economical. Among all the organic molecule-based catalysts, N-Heterocyclic Carbenes (NHCs) have evolved as the most promising catalysts for the oxidation of aldehydes to carboxylic acids.

Here in, we have developed a highly efficient triazolium-NHC-catalyzed method for the aerobic oxidation of aldehydes to the corresponding carboxylic acids under mild conditions in a short reaction time. More significantly, this method is suitable for several classes of challenging aldehydes such as ortho-substituted aryl aldehydes, highly electron-rich aryl aldehydes and indole-3-carboxaldehydes. We have also demonstrated this method for a gram-scale synthesis.

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PP-23

An Introduction and Updates to Greenhouse Effect, Greenhouse Gases and Global Warming

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The earth's climate is changing regularly. Warming of Earth's surface called greenhouse effect is a complicated natural phenomenon and vital to life as it maintains earth's average temperature of 15^0C, a more hospitable instead of -18^0C. The process of greenhouse effect involves sunlight, some gases and particles in the atmosphere. The greenhouse gases absorb some of the heat energy that escapes to the space and led to the warming of earth's lower atmosphere. An increase in the concentration of greenhouse gases may lead to problems. The present article is an introduction and updates to the concept of greenhouse effect, greenhouse gases global warming and its effect and measures to reduce global warming.

Keywords: Greenhouse Effect. Greenhouse Gases, Global Warming

PP-24

Multicomponent One Pot Synthesis of Various Quinazoline and Quinazolinone Derivatives with the Help of Isatoic Anhydride as One of the Component

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Multicomponent reactions have always been an attractive and efficient synthesis strategy for the synthesis of organic compounds. Since the reaction is carried out in one step the yield obtained is great and at the same time the reduction in the number of steps makes it an efficient and green process. Isatoic anhydride serves as an important component in these MCR_S for the synthesis of these heterocyclic compounds. Here a review of the one pot reactions carried out with the help of isatoic anhydride for the synthesis of various mono, (2-substituted, 3-substituted) di (2, 3 di substituted) and other 2, 3 dihydroquinazolinones is given. The isatoic anhydride gets cyclocondenced with the other components of the reaction and produces various quinazolines and quinazolinone derivatives.diffrent substitutions in the isatoic anhydride unit brigs the variety of differently substituted product range. The pharmacological importance of this class of heterocyclic compound is well known and is being explored as a promising potent biologically active compound. These compounds are of immense importance to the medicinal and therapeutic field and are widely used in various drugs to cure a number of diseases.

Keywords: Multicomponent Reactions, Isatoic Anhydride, Quinazoline, Quinazolinone

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PP-25

Review on Green Synthesis of Copper Nanoparticles using Microorganisms

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In recent years, nanotechnology or nanoscience is the fastest growing area of science and research. It deals with the particles having one dimension of about 1-100 nm range. The studies and applications of nanoparticles are widely used in various fields like academic, engineering, biology, agriculture, pharmaceuticals, medicine etc. The biosynthesis of nanoparticles from microorganisms (like bacteria, fungi, algae, yeast, and viruses) is thought to be nontoxic, eco-friendly and environmentally acceptable “green chemistry” approaches. This field has received great attention due to its capability to design alternative, safer, energy efficient, and less toxic routes towards synthesis. The application of the twelve principles of green chemistry in nanoparticles synthesis is a comparatively new emerging issue pertaining to the sustainable development. The present study includes both the intracellular or extracellular route for the production of copper nanoparticles. There is a need to summarize the behavior of copper nanoparticles in different media under various conditions. In this review, we compared Cu NPs with the others metallic NPs on the basis of catalytic activity, stability and conductivity.

PP-26

On The Microwave Synthesis and Characterisation of Some New Transition Metal Complexes with Acyl Hydrazine and Hydrazones

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A Series of sterically hindered complexes of CuII, CoII, MnII, NiII with O, N donor Acyl hydrazine and hydrazones; [M(BIH)2]X, [M(INH)2]X, [M(BBH)2]X, [M(BH)2]X and [M(SH)2]X where X= SO42-; M = CuII, CoII, MnII, NiII have been synthesised and characterized by Infrared, Magnetic measurements and UV-Vis spectral studies.

Keywords: Acyl Hydrazine, Hydrazones, Infrared, UV-Visible Spectra, Transition Metal

PP-27

Ameliorative Effect of Ziziphus Jujuba on Sodium Arsenite Induced Toxicity in Charles Foster Rats

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Introduction: In the recent times, arsenic poisoning in the ground water in the plains of the Gangetic basin has increased many folds. It is estimated that more than 200 million population in the Ganga Meghna Brahmaputra (GMB) plains are affected due to arsenic poisoning. This has caused severe health hazards in the exposed population. In Bihar, about 18 districts out of 39 are severely affected with arsenic poisoning in ground water. The exposed population are exhibiting the typical symptoms of arsenicosis denotes the magnitude of the exposure. Hence, the present study is focused to combat the deleterious effect of arsenic toxicity in animal models utilizing medicinal plant extract.

Methods: They animals (Charles Foster rats) were treated with Sodium arsenite at the dose of 8 mg per kg body weight for 16 weeks to make arsenic model and upon these arsenic pre-treated rats seed extracts of Ziziphus jujuba at the dose of 250 mg per kg body weight was administered for 4 weeks to study the ameliorative effects of this plant extract. After the entire treatment, rats were sacrificed and their blood samples were obtained and analysed for haematological and biochemical study while their tissues like liver and kidney were fixed in the respective fixative for the histopathological study.

Results: The study shows that arsenic induced toxicity caused deleterious effect on the rats at the haematological, biochemical and histopathological levels, but there was significant normalisation in the animal at all the respective levels.

Discussion: The arsenic causes deleterious effect in rats at heamotological, biochemical and histopathological level but the plant extract of Ziziphus jujuba played the vital role in the normalisation of these effects. Hence, it possesses ameliorative properties against arsenic induced toxicity.

Keywords: Sodium Arsenite, Ziziphus Jujujba, Amelerioative Effect, Rats

PP-28

Herbal and Traditional Medicines

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Herbal medicines are naturally occurring, plant-derived substances that are used to treat illness within local or regional healing practices. These products are complex mixture organic chemicals that come from any raw or processed part of a plant. Herbal medicine also called botanical medicine, use the plant's seed, berries, roots, leaves, or flower's for medicinal purpose. Herbal product's and traditional medicine are of great importance such form of medicine as traditional Chinese medicine, Ayurveda, Kampo, Traditional Korean Medicine and Unani have been practiced in some area of the world and are developed from plant or plant part. Although only a tiny fraction of existing plant species have been scientifically researched for bioactivities since 1805 when the first pharmacologically active compound morphine was isolated from Opium. Herbal medicines are considerable as a favorable future medicine for the management of healthcare.

PP-29

Impact of Diclofenac Sodium on Protein Content of Zebra Fish, Danio Rerio

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Diclofenac a non-steroidal anti-inflammatory drug is one of the most predominant pharmaceutically active compound which directly or indirectly enters into aquatic environment and shows negative impact on non targeted species such as fishes. In this context the toxicity evaluation of diclofenac sodium is under taken on protein concentration of fresh water fish *Danio rerio*. LC50 at 96 hrs exposure of diclofenac determined by direct interpolation method, was found to be 11.25mg/l. For the estimation of protein content fishes were divided into four separate groups of ten fish each. First group served as control, second group exposed with 96 hrs LC50. Third and fourth groups treated with 1/5 of LC50 of 96 hrs for seven and fifteen days respectively. After the completion of the experiment fishes were sacrificed to estimate the protein concentration in liver, gills and muscles. It was noticed that protein concentration of liver and muscles of the fish decreased within 24 hrs diclofenac exposure. In gills there was marked increase in 7 day exposure but decreased level was observed in 24 and 15 days. This study reveals that diclofenac can alter the level of the protein in fishes.

Keywords: Diclofenac (DCF), Toxicity, Zebra Fish, Protein Content, LC50

PP-30

Waste Water Management by Modified Guar Gum

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The growing concern towards the non-toxic, bio-compatible, biodegradable and renewable substances evolution, more accent has been given to natural polysaccharides. Guar gum is an inexpensive naturally occurring polysaccharide which is bio-compatible, biodegradable and non-toxic. It consist of a backbone of 1,4- linked β-D-mannopyranosyl units with branches of 1,6- linked α-D-galactopyranosyl units. Since there are primary and secondary hydroxyl groups on its backbone, it can be easily chemically modified to improve its physio-chemical properties. In recent years, guar gum and it's derivatives have emerged as promising bio-

material for various applications such as drug delivery system, tissue engineering scaffolds, bio-sensors, anti-microbial agent, wound healing material, explosives, food industry, agriculture, textile, paper industry, pharmaceutical and medical industry, cosmetics, water treatment (dye and heavy metal ion removal) etc. Here, we report the waste water management by the application of modified guar gum. Utilization of Guar gum based hydrogel and nanocomposite material has been elaborated in this work.

PP-31

Microwave Assisted Synthesis of 2-aryl-1-(arylmethyl)-1*H*-benzimidazoles Derivatives

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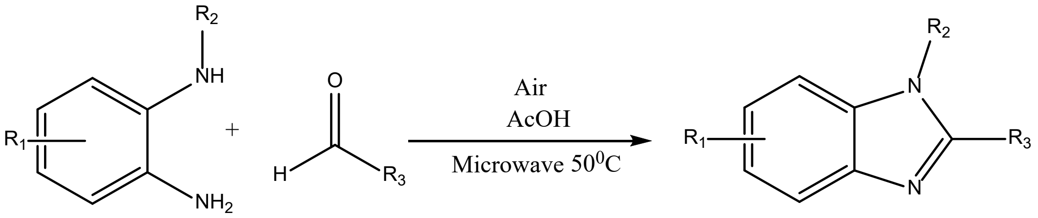
To minimize the use and generation of hazardous substances various eco-friendly, renewable, efficient, facile processes and design of products are encouraging. Microwave assisted reactions, one of them are much convenient because these proceed via fast rate of reaction, high yield and cleaner product. For this purpose the synthesis of 2-aryl-1-(arylmethyl)-1*H*-benzimidazoles under microwave irradiation and thermal condition proceed via condensation of phenylenediamine with aldehyde in acetic acid. Benzimidazole derivatives are applicable as anthelminthic agents, selective neuropeptide YY1 receptor antagonists[2], 5-lipoxygenase inhibitors[3], human cytomegalovirus (HCMV) inhibitors[4], and poly (ADP-ribose) polymerase (PARP) inhibitors[5] etc.

Keywords: Benzimidazole, Receptor Antagonists, HCMV, PARP



Scheme 1 Synthesis of Benzimidazole under Microwave Irradiation
(Where R_1= EDG; R_2=H, alkyl; R_3= EDG)

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PP-32

Synthesis and Biological Activity of Quinazoline-4-(3H)-One Derivatives

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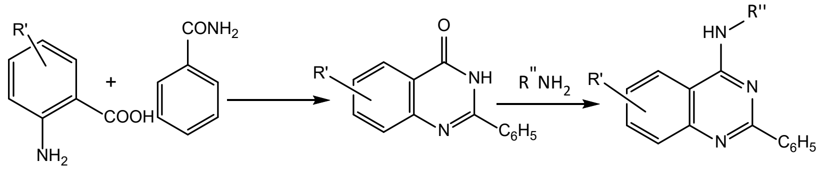
Quinozolinone, N-containing heterocyclic compounds, comprise a vast array of biologically active compounds ubiquitous in plants, many of which have been used in traditional medicine since ancient times for distinct biopharmaceutical activities. Reaction of the anthranilic acid and different acid derivatives form new quinazolinone series [1]. These derivatives show various biological activities such as antimicrobial[2] and anticancerous activities[3]. There are more than 150 naturally occurig alkaloides, known for anti-leishmanial agents, anti-convulsant, sedative, hypnotic, analgesic, antidiabetic, anti-inflammatory, anti-tumor properties [4] consists of Quinazolinone and their derivatives. The synthetic method is shown in scheme 1. Quinazolinone derivatives are the emerging pharmacophore which has drawn a growing interest in the arena of drug designing.

Keywords: Anti-Leishmanial, Quinazolinone, Antifungal, Antibacterial, Anticancerous



R'=H, Alkyl,EDG
R''=Phenyl, Styryl, Phthalimido methyl,Benzamidomethyl

Scheme 1 Condensation of Anthranilic Acids with Primary Amines

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PP-33

Global Warming: Consquences and Remedial Measures

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Global warming which occurs due to greenhouse effect is a big problem in today's society and everyone will soon have to face it. As a result of human activities greenhouse gases accumulate in earth's atmosphere and trap heat that escape to the space, causing temperature to rise. In recent past, the average global temperature has increased at the fastest rate and the trend is accelerating. Global warming is believed to be permanently changing earth's climate. The present paper summarizes the consequences of global warming and remedial measures to reduce emissions of greenhouse gases.

Keywords: Global Warming, Greenhouse Gases

PP-34

Detection of Chlorofluorocarbons (CFCs) and Carbon Tetrachloride (CCl4) in the Air with Help of One Dimensional Photonic Crystal Device

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In this work, we have proposed an idea to detect the Chlorofluorocarbons (CFCs) and Carbon tetrachloride (CCl4) in the air with help of one dimensional photonic crystal (1DPC) device which is composed of dielectric materials. The detection of CFC and CCl4 is based on the shifting of defect wavelength peak obtained in the transmission spectra on the 1DPC. The transmission of 1DPC was calculated using transfer matrix method (TMM) on considering the normal incidence angle on the surface. The transmission spectra of different filling fractions of CFC and CCl4 in the air medium give tunability of defect peak wavelength which is help to detect these gases.

PP-35

Synthetic Applications of O-Substituted Hydroxylamines

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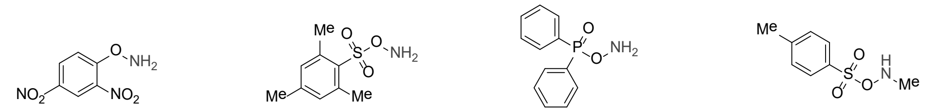
O-Substituted hydroxylamine derivatives like O-(diphenyl phosphinyl)hydroxylamine (DPPH), O-(Mesitylsulfonyl) hydroxylamine (MSH), 2,4-Dinitrophenylhydroxylamine (DPH) and other analogous reagents in which oxygen is substituted with good leaving group, have great potential for amination reaction. These aminating reagents provide stereo- and regioselective C-N, N-N, O-N, and S-N bond formation reactions with or without metal catalyst. Herein we are unfolding the synthetic applications of various O-substituted hydroxylamines.1-5

Some selected examples of O-Substitutedhydroxyl amines



1 2·4-dinitrophenylhydroxylamine (DPH)

2 O-(mesitylsulfonyl)hydroxylamine (MSH)

3 O-(diphenylphosphinyl)hydroxyamine (DPPH)

4 N-methyl-O-tosylhydroxylamine (TsONHMe)

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PP-36

N-H Aziridination of Enones

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Enone aziridines are present in varieties of natural product and bio active molecules. These aziridines are also important synthetic intermediate, as they can easily convert into amino alcohols, di-amines, amino-thiols etc. via SN2 ring opening. Most of the enones aziridines were prepared by the using of substituted hydroxyl amines as aminating reagent. Herein we are describe the various methods for the synthesis of enone aziridines by substituted hydroxyl amines.[1]

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PP-37

Comparative Study of Oxidation of D-Mannitol and D-Sorbitol by Sodium N-Chloro-p-toluenesulfonamide using Chloro-complex of Ir(III) in its Nano-concentration Range as Homogeneous Catalyst: A Kinetic and Mechanistic Investigations

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The kinetics and mechanism of homogeneously Ir(III) chloride catalyzed oxidation of D-Mannitol and D-Sorbitol by Sodium N-Chloro-p-toluenesulfonamide [CAT] have been investigated in perchloric acidic medium in presence of mercuric acetate as a scavenger in the temperature range 30 °C – 45 °C. The reactions follow identical kinetics. The experimental results show first order kinetics with respect to the oxidant [CAT] and

catalyst [Ir(III)] while zero order with respect to both of the polyhydric alcohols were observed. The reaction shows negligible effect of [$Hg(OAc)_2$], [H^+] and ionic strength (μ) of the medium. Chloride ion positively influenced the rate of reaction. The reaction between chloramine-T and substrates (D-mannitol and D-Sorbitol) in acid medium shows 2:1 stoichiometry. To calculate activation parameters, the reactions have been studied at four different temperatures between 30 to 45 °C. A mechanism involving the complex formation between catalyst and oxidant has been proposed. D-Mannonic acid and D-Gluconic acid have been identified chromatographically and spectroscopically as the final product of oxidation of D-Mannitol and D-Sorbitol respectively. Based on the kinetic data, reaction stoichiometry and product analysis, a reaction mechanism has been proposed and rate law has been derived.

Keywords: Kinetics, Mechanism, Ir(III) Catalysis, Polyhydric Alcohols, Chloramine-T, Acidic Medium

PP-38

Microwave Radiation Assisted Synthesis of Serotonin (5-HT$_{1A}$ / 5-HT$_7$) Receptor Ligands

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Objective: Serotonin (5-hydroxytryptamine, 5-HT) is a neurotransmitter that mediates its effects on the central and peripheral nervous systems via interaction with 5-HT receptors. Due to its entanglement in the various psychiatric disorders such as anxiety and depression it is a subject of consummate research. Besides that, a subunit of serotonin i.e. 5-HT7 receptor plays a key role in learning and memory. Here we are presenting a microwave assisted synthesis of serotonin receptor ligands which minimizes the use of solvent.

Methods: This method allows the synthesis of 5-HT1A or 5-HT7 receptor ligands containing arylpiperazine moiety in increased yield, with lesser reaction time, using solvent-free conditions, assisted via microwave irradiation at reduced temperature in the presence of phase transfer catalyst.

Result and Discussion: Synthesized serotonin receptor ligands were prepared using environmental friendly conditions with minimal solvent usage which reduces toxicity. In addition reaction yield also improved and leads to increased cost effectiveness.

Conclusion: The synthesized ligands were prepared in high yield within short duration using green chemistry. The reported synthetic methodology doesn't require expensive and toxic reagents used for the synthesis of previously reported 5-HT1A or 5-HT7 receptor ligands. Henceforth the designed compound can serves as a facile and high yielding process for either 5-HT1A or 5-HT7.

PP-39

Green Synthesis of Third Generation TSPO Ligand

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Objective: TSPO, firstly described as peripheral benzodiazepine receptor (PBR) is an 18kDa protein, recognized as an important target for imaging the neuroinflammation using positron emission tomography (PET). TSPO ligands mainly used for the in vivo imaging and to detect activation of microglia, and have proven to be useful as noninvasive molecular imaging tool to assess neuroinflammation. Herein, we are reporting an ecofriendly method for the synthesis of third generation TSPO ligand which belongs to acetamidobenzoxazolone family.

Method: Proposed ligand will be synthesized with the use of 5-bromobenzo[d]oxazole-2(3H)-one and 3-methoxyphenyl boronic acid through Suzuki coupling reaction under microwave irradiation in presence of water as a solvent.

Results and Discussion: The proposed Acetamidobenzoxazolone derivative will be synthesized in high yield and will exhibit unique and effective binding affinity and selectivity towards the target protein (TSPO). The best advantage of this method is use of non-toxic reagents and green solvent. The practice of water as solvent features many benefits such as improving reactivity and selectivity, simplifying the workup procedures, enabling the recycling of the catalyst and allowing mild reaction conditions.

Conclusion: Compared with previously described approaches, our novel and environment friendly method will reduce overall reaction time without affecting reaction yield. The Benzoxazolone based derivative will serve as a promising TSPO selective ligand and its future applicability will be analyzed after various animals and human studies.

PP-40

CuNPs Catalyzed Green Synthesis of Triazoles

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Green Chemistry practices enables the synthesis safer and sustainable with less or no wastage discharge. Among its various aspects, nanocatalyst has occupied a peculiar position in green synthesis due to high surface area and working in water as solvent. Nanocatalysis is a green chemistry resource which can increases the inherent

effectiveness of copper-catalyzed azide-alkyne cycloaddition because of the enhanced catalytic activity of nanostructured metals and their admirable reutilization capability as heterogeneous catalysts. 1,2,3-triazoles are main class of heterocycles due to their extensive range of biological properties such as antimicrobial, anticancer, anti-HIV, antifungal, antiviral, antibacterial, antitubercular, antidiabetic, antiepileptic, antiallergic behavior and they are also used as optical brightness, light stabilizers, fluorescence chemosensors and corrosion retarding agents. 1,3-dipolar cycloaddtion between terminal alkynes and organic azides generating 1,4 disubstituted 1,2,3–triazoles has attracted considerable attention owing to its consistency, specificity and biocompatibility. Here the Synthesis of 1,4-disubstituted 1,2,3-triazoles by the use of CuNPs as a source of the heterogeneous catalytic species and water as solvent will be discussed.

Keywords: Green Chemistry, Nanocatalyst, Cycloaddition, Heterocycles, Triazoles

PP-41

Reinvestigation & Synthesis of Benzo-A-Pyrones Derivatives

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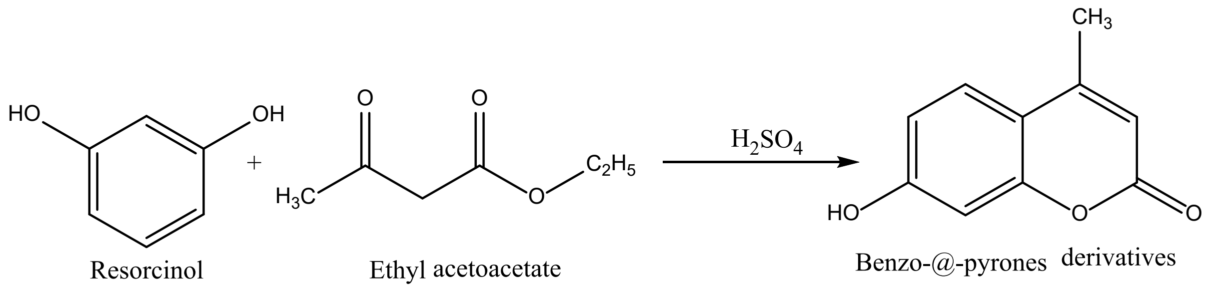
Benzo-α-pyrones also known as Coumarin derived from 'Coumarou', the vernacular name of the Tonka bean (*Dipteryx odorata*, wild Fabaceae family) from which it is first isolated in 1820[1]. It's derivatives are found at high level in some essential oil, cassia leaf oil,and Lavender oil. 2H-1-benzopyrano-2-one is a phenolic substance consists of fused benzene and α-pyrone ring. Classical synthesis of Coumarin derivative proceed via Claisen rearrangement, Perkin reaction, Pechmann reaction, wetting reaction as well as Knoevnagel condensation. Different Series of coumarin derivative has different biological activities like – Anti-Inflammatory Activity[2], Anti coagulant Activity[3], Antibacterial Activity, Anti fungal Activity, Antiviral Activity, Anticancer Activity[4], Anti-Hypertension Activity, Anti-Oxidant Activity, etc. Resorcinol react with ethyl acetoacetate in the presence of conc. Sulphuric acid for 18 hrs. to form 4-methyl-7- hydroxycoumarin[5].

Keywords: Benzo-α-pyrones, Anti-Inflammatory, Antibacterial Activity, Anti-Oxidant, etc.



Scheme: Synthesis of Benzo-α-pyrones Derivatives

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PP-42

Concise Way of Synthesis of Fe_2O_3 and Their Magnetic Behaviour

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The iron oxide nanoparticles have a great attraction in biomedical applications due to their non-toxic role in the biological systems. The uses of maghemite (γFe_2O_3) and magnetite(Fe_3O_4) nanoparticles, for an inhibition time in biological activities are listed in this work . This review explains the use of iron oxide nanoparticles in the biomedical fields with particular attention to the application of hematite and super paramagnetic iron oxide nano particles. This paper focuses on the synthesis, characteristics and biomedical applications of iron oxide nano particles. For most of their applications, the magnetic behaviour of iron oxide nanoparticles in a fluid is very important especially the high gradient magnetic separation of the particles from a non -magnetic liquid medium such as blood in the human body. From the review work the iron oxide nanoparticles may be specialised in particular bacterial and cancer treatment.

Keywords: Nanostructured Materials, Magnetic Fluid, Ultra Small Super Paramagnetic Iron Oxide

$$Fe^{2+} + 2Fe^{3+} + 8OH^{-} \longrightarrow Fe_3O_4 + 4H_2O$$

$$Fe_3O_4 + 2H^{+} \longrightarrow y\text{-}Fe_3O_4 + Fe^{2+} + H_2O$$

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PP-43

Synthesis and Characterization of Dibenzofuran Derivatives

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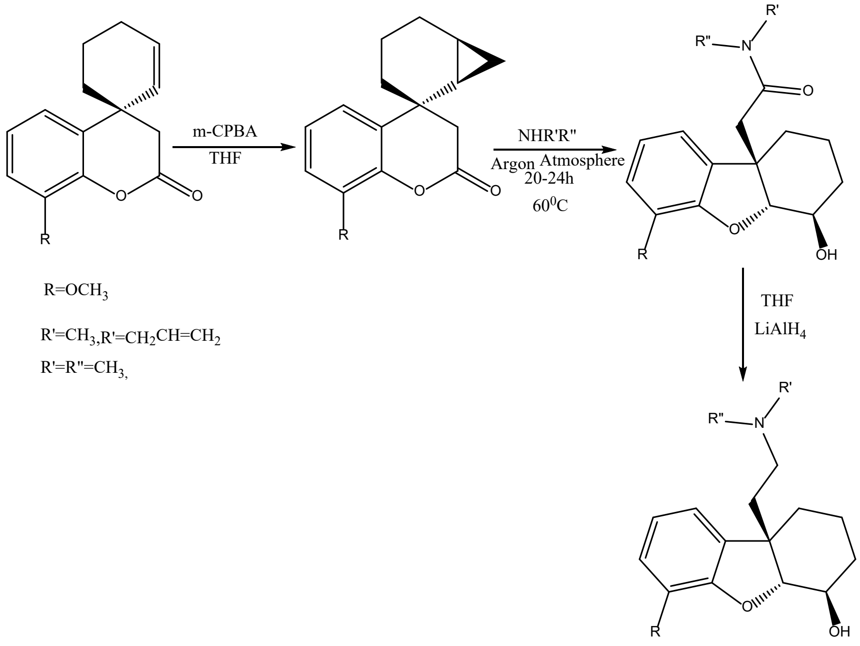
Dibenzofuran and its derivatives are well-known O-containing heterocyclic compounds exhibits important applications such as antibacterial, antifungal, antiviral, antioxidant, antimicrobial, anti-inflammatory, antiandrogenic [1], antitubercular [2], and antitumor [3] activities. A new series of coumarin based compound dibenzofuran have synthesized accomplishing high selectivity and potent effects with low nano-molar affinity against the tumor associated carbonyl anhydrase by displaying cytotoxic effect after 48 hrs of incubation in both mormoxic & hypoxic condition with cancer cell line. .Effective and straight forward route has been demonstrated for the synthesis of dibenzofurans derivatives via rearangement of a spirodihydrocoumarin[4] (Scheme). The present study shows that Benzofuran derivatives represent a promising class of multi-targeting derivatives which can interact with several biological targets, such as lipoxygenase and carbonic anhydrases.



Scheme: Synthesis of Dibenzofurans Derivatives via Rearangement of a Spirodihydrocoumarin

Keyword: Benzofuran, Coumarins, Anticancer, Carbonyl Anhydrase

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PP-44

Novel Multifunctional Porous Multilayered Materials with Different Compositions for Environment and Energy Applications

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In recent years, several synthetic techniques are using to synthesis the multilayered material of different compositions that is called one-dimensional multilayered material (ODMM). The synthesized ODMM, porosity and multilayered structure properties, may be a new device when the both basic concepts of thin film and surface physics are introduced. The structural origin of ODMM is developing to perform the useful optical properties of multilayered structure of different compositions [1]. Such optical materials possess a unique property called refractive index. The refractive indices of multilayered materials in periodically varies in the space are produced the interesting optical properties due to multiple interference at the interfaces of two materials. The optical properties of the multilayered material structures have analyzed theoretically by using transfer matrix method (TMM) with variation of optical parameters [2]. The potential applications of such multilayered optical material with one-dimensional structure of different compositions having high porosity may be used in the various fields related to energy and environmental sciences such as detection of ozone, chemical species, photovoltaic and sensor etc.

PP-45

Reinvestigation of Halogenation of Pinacolone at Ambient Temperature

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We reported here easiest methods for the a-halogenation of pinacolone by using reported procedure. These derivatives are highly lachrymatory compounds. Care was therefore taken in handling and the preparative procedures were followed in a properly ventilated fume cup-board. The used glass-wares were soaked in NaOH solution before washing.

The desired compounds were prepared from the respective parent ketones by the halogenation at α-carbon

$$t\text{-BuCOCH}_3 + Br_2 \xrightarrow{\text{Acetic acid}} t\text{-BuCOCH}_2Br + HBr$$

$$t\text{-BuCOCH}_3 + SO_2Cl_2 \xrightarrow[\text{at } 0^0\text{ C}]{\text{Diethy ether}} t\text{-BuCOCH}_2Cl + HCl$$

$$t\text{-BuCOCH}_2Cl + NaI \xrightarrow{\text{Diethy ether}} t\text{-BuCOCH}_2I + NaCl$$

In a general procedure, bromine (5.12 mL, 100 mmol) was added slowly from a pressure equalizing dropping funnel to a solution of pinacolone (100 mmol) in glacial acetic acid (~ 20 mL) with constant stirring. Flask was warmed by a hot air gun whenever required, for few minutes to initiate the reaction. During addition, the colour of bromine faded to straw yellow. Addition was completed in 10-15 minutes and the whole reaction mixture was poured into a beaker containing crushed ice. A yellow liquid settled at the bottom. [1]

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PP-46

A Facile Method to Fabricate High-Aspect Ratio ZnO Nanowires: Characterizations and its Application for Photocatalytic Degradation of Rhodamine B

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A facile and easy route is employed to synthesized highly crystalline solid- cylindrical ZnO nanowires by gradual addition of HMTA solution into the Zinc acetate solution under continuous stirring followed to the addition of SDS solution gradually with respect to time. The structural, morphological, and optical characterizations were successfully examined by XRD, FESEM, UV-Vis., FTIR and PL. The as-synthesized ZnO nanowires exhibited remarkable result as photocatalyst for facile degradation of Rhodamine B under UV- light illumination and it follows the 1st order kinetics and their rate constant were found to be k_{app} (0.01405 $mint^{-1}$).

Keywords: Nanowires, FESEM, UV-VIS, PL, Rh B & Photocatalysis

PP-47

Studies of Molecular Interactions in Binary Liquid Mixtures using Ultrasonic Techniques

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Ultrasonic velocity (u), density), and viscosity have been measured for binary liquid mixtures (Acetophenone + Cyclohexane) at 308K. The density) of the pure solvents and binary liquid mixtures were accurately determined by Magnetic Float Densitometer. It has been seen experimentally that for the same liquid, if the weight on the float is increased, corresponding current will decrease and vice versa. Thermo-acoustical parameters like adiabatic compressibility (β_{ad}), volume change (dV), free length (L_f), free volume (V_f) etc. have been computed from the experimental data. These computed values indicate the presence of specific types of molecular interaction involves between the liquid mixtures. Also, discussed these interactions such as dipole – dipole interaction and dipole—induced dipole interaction through hydrogen bonding occurring between components of mixtures. This provides a useful information about inter and intra molecular interactions of mixture existing in the liquid system.

Keywords: Ultrasonic Velocity, Density, Viscosity, Acoustical Parameters, Acetophenone, Cyclohexane, Molecular Interactions

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PP-48

Synthesis of CNT Doped Nano Material by Sol-Gel Method and its Application as Cathode Material

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The sample $Li_2Fe_{0.4}Mn_{0.6}SiO_4$ synthesized via sol-gel method and MWCNT was deposited by solution cast method. Synthesized material was investigated using various characterization techniques like FESEM, EDS, Impedance analysis, CV and CP. The FESEM exhibits the particle size as 24 nm for 9 weight% which is less compared to bulk sample of $Li_2Fe_{0.4}Mn_{0.6}SiO_{4.}$ Conductivity was observed in the order of 10^{-3} which is 3 order enhance as compare to as synthesized $Li_2Fe_{0.4}Mn_{0.6}SiO_{4.}$ CV results show the capacity in terms of power which is maximum as 92.0 mW/g for CNT-9 weight%. The capacity retention, found that the maximum discharge capacity retains for 9 wt% doping of carbon nano tube. 9 wt% content of MWCNT in Li2Fe0.4Mn0.6SiO4 material is one of the best candidate for making nano composite cathode material for the Li-ion batteries.

Keywords: $Li_2Fe_{0.4}Mn_{0.6}SiO_4$, Electrical Conductivity

PP-49

Innovative Synthesis of Thiophene and its Derivatives

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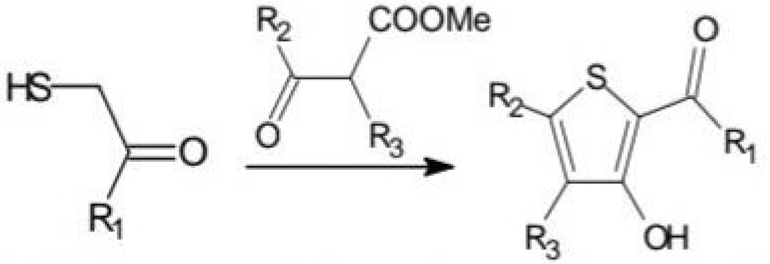
Thiophene nucleus has been established as the potential entity in the largely growing chemical world of heterocyclic compounds possessing promising pharmacological characteristics. The similar compounds synthesized through different routes bear variable magnitudes of biological activities. The knowledge of various synthetic pathways and the diverse physicochemical parameters of such compounds draw the especial attention of medicinal chemists to produce combinatorial library and carry out exhaustive efforts in the search of lead molecules. In medicinal chemistry, thiophene derivatives have been very well known for their therapeutic applications. Many thiophene derivatives have been developed as chemotherapeutic agents andare widely used.

Keywords: Condensation reaction of thioglycolic acid with α, β- acetylenic esters, which upon treatmentwith base result in the formation of 3- hydroxyl- 2- thiophenecarboxylic acid[1]. Fiesselmann Thiophene Synthesis is an extension of Woodward condensation of thioglycolic acid [2] and α, β- unsaturated ester in the presence of base to produce 2-carbomethoxy-3- ketotetrahydrothiophene.

Scheme:



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PP-50

Nanostructured Spherical-shaped Sc(III) Polyacrylate for Monitoring the Moisture Level

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The present paper reports the investigation of transmitted power through the nanostructured scandium polyacrylate (Sc(III) PAcr) deposited on flat borosilicate substrates to examine the adsorption/desorption of humidity at room temperature. For this purpose, the precursor of Sc(CH2=CH-COO)3 was prepared and used for film deposition. The film was then investigated using SEM and UV–Vis absorption techniques. Scanning Electron Microscope showed the spherical shaped clusters of the material. Energy band-gap of the film was estimated as 3.887 eV by UV–Vis spectrophotometer. Transmission Electron Microscope revealed the minimum grain diameter of ~21 nm and SAED showed its polycrystalline nature. From Zeta nanosizer, minimum particle size was found as 18 nm. FTIR confirmed the bond formation in the material. The surface area analysis shows that the pore volume of Sc(III) PAcr is 0.15 cm3/g which is quite small whereas the surface area and mean pore radius of the spherical structure are 60.1 m2/g and 41.2 Å respectively. The film was employed as transmission based opto-electronic humidity sensor. Maximum sensitivity was found as 2.1 μW/%RH with 89% reproducibility. Response and recovery times of the sensor were found as 25 s and 155 s respectively.

Keywords: Humidity, Metallopolymer, Polyacrylate, Scandium, Sensor

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PP-51

Recent Development of Gas Sensors by Using Metal Oxide based Heterostructures, their Future Opportunities and Challenges: A Review

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In recent time, atmospheric pollution has become a critical problem for modern society. These pollutants basically contain hazardous gases. Their detection and monitoring have become a major problem for researchers. Metal oxides play a vital role in the detection of different gases owing to their change in electrical or optical parameters relative to the adsorption/desorption of gas. The combination of different metal oxides forms heterostructures. The sensitivity and selectivity of these sensors have been improved by incorporation of heterostructures. Heterostructures may improve sensor performance through facilitating catalytic activity, increasing adsorption and creating a charge carrier depletion layer that produces a larger modulation in resistance. This article reviews various fabrication methods which seem to be very efficient to obtain metal oxide-based heterostructures with different morphologies and dimensions. The heterostructures posses different types of structures such as core-shell, one-dimensional, two-dimensional and three-dimensional, hence improves the important sensing parameters of the sensor. A compositional contribution of an individual metal oxide within a composite exhibits the capability to tune the composite's response and selectivity towards a particular gas.

Keywords: Metal Oxides; Heterostructures; Gas Sensing

PP-52

Synthesis of MWCNT/PPY Nanocomposite Using Oxidation Polymerization Method and its Application as CO_2 Sensor

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The composite based on multiwall carbon nanotube (MWCNT) and conducting polymer polypyrrole (PPY) are promising material for gas and humidity sensing due to their unique nanostructure. The MWCNT was prepared by using direct liquid injection chemical vapor deposition technique (DLICVD) and MWCNT/PPY based nanocomposite was synthesized by the oxidation polymerization method. The thin film of MWCNT/PPY was prepared by spin coating technique and characterized using scanning electron microscope (SEM), Tunneling electron microscope (TEM), Particle size analyzer and X-ray diffractometer (XRD). The vibrational and rotational spectroscopy was observed through Fourier Transform Infrared Spectroscopy (FTIR) and Raman spectroscopy. The optical band gap was found to be 3.27 eV and the minimum crystallite size was found to be 8 nm. The synthesized MWCNT/PPY has been used for CO_2 and humidity sensing. The sensor response and sensitivity of thin film towards CO_2 was found to be 2.629 and 39 kΩ/sec respectively at 2 vol%.

Keywords: MWCNT, DLICVD, CO_2 Sensor

PP-53

Synthesis and Characterization of ZnO Quantum Dots and its Application as Electrical Humidity Sensor

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The present paper reports the synthesis and characterization of ZnO quantum dots. It was synthesized via Colloidal (solution) method with oleic acid (OA) as the surface-capping ligand. The well dispersed ZnO quantum dots were fabricated on glass substrates by using the spin coating method. The fabricated film was investigated through the Scanning Electron Microscope (SEM), X-ray diffraction (XRD), transsmision electron microscopy (TEM) and UV–Vis absorption techniques. XRD revealed the crystalline nature of the quantum dot and evaluated the average nanocrystalline size was found to be 20 nm. The energy band gap was calculated from UV–Vis absorption that is 3.5 eV. TEM image showed the size of the dots 0.69-2.5 nm. Colloidal quantum dots (CQDs) have excellent properties like as low cost and environmental friendly, that is applicable for humidity sensors. The Maximum sensitivity was found as~ 13.03 MΩ. Response and recovery times were found as 6 s and 48 s respectively. The experiments were repeated time to time and reproducibility was found ~95% with negligible ageing effect.

Keywords: Quantum Dot, Electrical Humidity Sensor, Solution Method

PP-54

Synthesis and Characterization of Zno/ Mgo Nanohybrid Nanomaterial for Sensing Application

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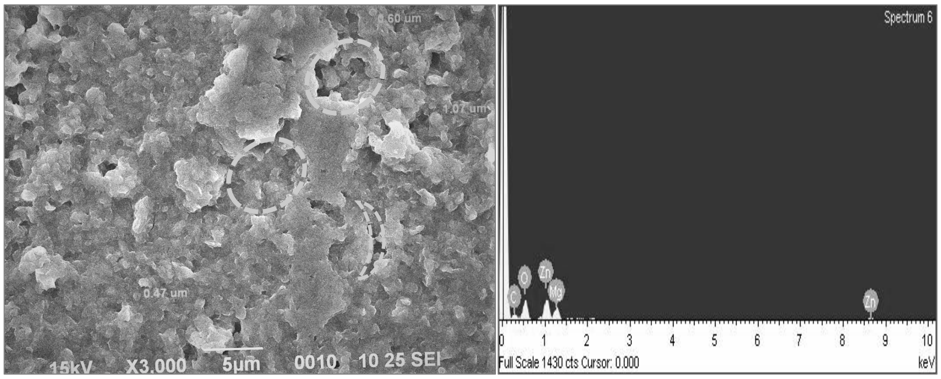
ZnO/MgO nanohybrid material synthesized by single step sol-gel method. For the humidity sensor application the film was fabricated using spin coating technique. The surface morphological investigated using SEM analysis. Crystalline nature was confirmed by X-ray diffraction, revealing its average and minimum crystallite size of the material. Physical properties like surface area, particle size, optical absorbance and thermal stability of as fabricated thin film were deeply investigated using BET, Particle size analysis, UV absorption, FTIR analysis respectively. Humidity sensing characteristics were tested by analyzing capacitive performance of ZnO/MgO nanohybrid based humidity sensor. Thus ZnO/MgO nanohybrid based capacitive humidity sensor ensures its potential towards the reliable and safer use in the detection of humidity.

Keywords: Hybrid Material, Capacitive Humidity Sensor, Characterization



PP-55

Biodiesel: An Economical and Eco-friendly Renewable Fuel for Future

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A process for the production of biodiesel as an efficient fuel from non-edible oil has been studied. The essential part of the process is the transesterification of the used industrial waste oil using base as a catalyst and an alcohol (methanol) to get an ester of the respective biodiesel as a product and glycerol a by-product. It consists of non-edible oil and belongs to ecological fuels because of the qualitative composition (carbon 77%, hydrogen 12% and oxygen 11%). Biodiesel fuel produces no net output of carbon in the form of CO_2, as the oil crops absorb the same amount of CO_2 as is released when the biodiesel combusted. Biodiesel is a nontoxic, biodegradable and renewable source of energy. Environmental benefits of its use include lower exhaust emission of particulate matter and green house gases, such as CO, CO_2 and SO_x. Biodiesel is a environmentally friendly biofuel since it provides a means to recycle CO_2, biodiesel does not contribute to global warming. Perhaps the next most critical pollutant from the perspectives of human health and environmental quality is NO_x; NO_x is the key to controlling ground level ozone and smog in urban areas.

Keyword: Biodiesel, Transesterification, Nontoxic and Environment Friendly Fuel

Average biodiesel emission compared to petroleum diesel according to Environmental Protection Agency

Emission	B100	B20
Carbon monoxide	-48	-12
Total unburned hydrocarbons	-67	-20
Particulate matter	-47	-12
Nitrogen oxides	+10	+2
Sulphates	-100	-20
Air toxics	-60 to -90	-12 to -20

PP-56

Ionic Liquids Recyclable, Efficient, Potential Green Solvent and Catalyst in One-pot Conversions

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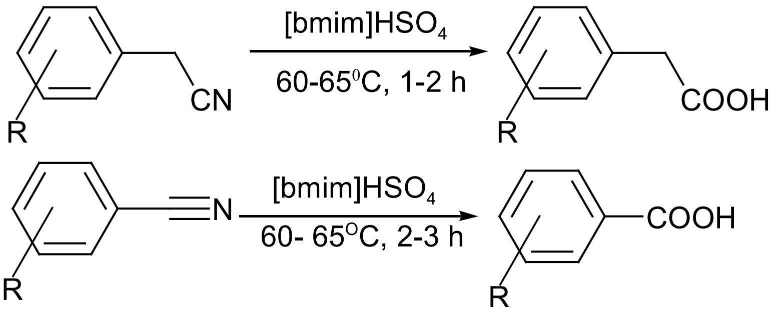
Green approaches found due respect for the synthesis of number of important complex products or intermediate/precursors, as they are environment benign and human friendly in nature. Moreover conversion techniques are important synthetic tool in organic chemistry and in the voyage of conversion of nitriles to carboxylic acid a variety of methods have been develop till date. Some of them required drastic conditions, involving hydrolysis of nitriles in either strong acidic or basic medium at elevated temperature under elongated stirring time.[1-3] While others entail two step hydrolysis protocols, via formation of amides and their conversion to corresponding acids[4]. In addition to this use of sodium perborate and copper salts in heterogeneous medium at higher temperature[5] is also well documented. But all aforementioned approaches involve use of hazardous chemicals and tedious process which were found to have their own shortcoming of side product formation and low product yield along with health hazard.

To overcome these, cumbersome Green approach was envisaged, in which various enzymes such as nitrilase hydratase, amidase and nitrilase were used for the conversion of nitriles into acids.[6]

Further ionic liquids have attracted considerable attention of chemist for their use as an efficient and green solvent for large number of chemical reactions[7]. Moreover, the use of ionic liquids is environmentally benign and reduces the use of toxic chemicals and reaction time significantly[8]. Importantly, ionic liquid are very efficient and clean which give selectivity and quantitatively single product in the reaction, hence, no purification of product is needed.

In continuation of the above green approach “our research group” is exploring the chemistry of Ionic liquids as an efficient green catalyst and solvent system for conversion reactions. After exploring number of ionic liquids we selected [bmim]HSO_4 ionic liquid as an efficient and effective catalyst/solvent system for the single step conversion of nitriles into corresponding carboxylic acid. The reaction condition are mild involves heating of nitriles containing [bmim]HSO_4 at 60-65°C for 1-3 hours to give quantitatively (80-96%) pure products. The ionic liquid was recovered and reused. The protocols are applicable for both aromatic as well as aliphatic nitriles having various substituents and were found equally sensitive towards transformation in the ionic liquid and final product yields.



General Scheme: Conversion of Nitrile into Carboxylic acid via Ionic liquid [bmim]HSO_4

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PP-57

An Overview of Green Approaches towards the Synthesis of Flavone Scaffold

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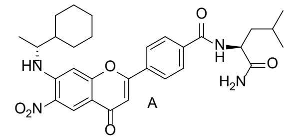
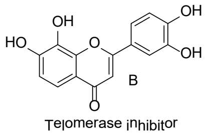
Green chemistry focusses on the reduction of pollution at Source, thus ensures the environmental safety and conservation of energy and raw materials. Crafting the traditional synthetic organic routes to less-hazardous environmentally benign transformations is the recent trend in organic chemistry. Different approaches to green a reaction include reduction of synthetic steps, run-through of greener solvents and catalysts and use of renewable resources and energy. Flavone, also named as 4-phenyl chromone, is a member of oxygen heterocyclic family 'flavonoids' that found extensively in nature and is well identified privileged structure in drug discovery and development. Anti-oxidant property of flavones are well known, in addition it exhibit anti-cancer, anti-hypertensive, anti-HIV, anti-inflammatory antimicrobials, anti-arrhythmic and antiulcer properties. For example compound (A) shows anti-cancer activity, compound (B) acts as telomerase inhibitor and compound (C) shows tropomyosin-receptor agonist property. A huge number of synthesis, transformation and functionalization of this valuable moiety is present in literature. Thus, herein, we present an overview of environment friendly protocols adopted to synthesize flavone nucleus.

Keywords: Green Synthesis, Flavone, Chromone, Solvent Free Synthesis



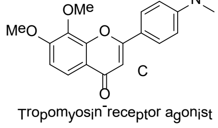
A

Anticancer agent



B

Telomerase inhibitor



C

Tropomyosin-receptor agonist

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PP-58

Utilization of Biological Fauna for Plastics bio-degradation

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Science is frantically searching for better alternative to replace plastics. While products made from corn-starch, paper and other plant-based materials are good substitutes, but the production of these materials is expensive and is unable to meet the enormous demand. According to the W.H.O, “Once dioxins have entered the environment or body, they are there to stay due to their uncanny ability to dissolve in fats and to their rock-solid chemical stability”. That’s why; still, plastic is biggest problem around us. An accidental discovery has raised hopes to find a parallel solution to the problem of breaking down plastic. Federica Bertocchini, a researcher at the Spanish National Research Council and team of a Scientist at Cambridge University, found a type of worms that eat plastic. Naturally, a poly-bag degrades in 400-500 years. Experimental studies revealed that about 100 worms can degrade 92 milligrams of polyethylene in just 12 hours.

Keywords: Plastic, Biodegradation, Galleria Mellonella

PP-59

Green Synthesis of Silver Nanoparticle by Using Flower Extract

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Silver nano particle has impressive application in the field of medicine as antimicrobial agent and these are eco-friendly. The parts of different plants used for the synthesis of nano particles is considered as a green technology. This technology is one of the best eco-friendly method and does not show any harmful effect. In India over more than 6000 plants are used in the traditional, mythology and herbal medicine. The Indian system of medicine has found 1500 medicinal plants in which 500 are commonly used. There are several flower plant extract by which silver nano particle is synthesized by green method. These flower extract such as *Hibicus Rosa sinesis, Caledula officinalis* commonly called as *marigold, Ixora coccinea and cassia auriculata*. The synthesis of silver nano particles occurred under the exposure of the flower extract to 1mm-5mm silver nitrate solution. During this process the complete reduction of silver nitrate was observed nearly 48 hours of reaction at 30^{0}C under vigorous shaking conditions. The formation of silver nano particles is made confirmed by FT-IR, UV-Visible, TLC and Scanning electron microscopy (SEM). These showed that the particles were capped with the bimolecular compounds like terpenoids, amino acids, proteins, alkaloids. SEM analysis showed the particle size between 5-40 nm and spherical in structure.

PP-60

New Generation Eco Green Materials: A Review

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The idea of new generation eco-green materials incorporates a variety of approaches during the manufacturing, period of design, maintenance and operation of materials. The motive of this study aims at examining eco-friendly product quality and eco-friendly preference on the environment and their impact on customer satisfaction. So, it's today need to achieve good manufacturing practices and energy efficient material which help in less production of greenhouse gases and save energy. The manufactured material must be easily biodegradable, reusable, reducible and recyclable. For example, the construction industry is heightening abruptly and new technologies have evolved very fast to accommodate various obstacles in the construction industries. Concrete is the primary materials for construction purposes among all materials used in construction industries. The production of concrete is done by mining tons of naturally occurring materials which will leave a significant impact on the environment. Nowadays recycling of industrial by-product and waste gaining popularity to make concrete eco green material and the concrete can be called as Green concrete.

Keywords: New Generation Eco-green Materials, Biodegradable, Reusable, Reducible and Recyclable

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PP-61

Pollution Prevention

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Pollution is the contamination of air, soil, or water by the discharge of harmful substances. Pollution prevention is the reduction or elimination of pollution at the source instead of at the end-of-the-pipe or stack. Pollution prevention occurs when the raw materials, water, energy and other resources are utilized more efficiently, when less harmful substances are substituted for hazardous ones and when toxic substances are eliminated from the production process. Source reduction allows for the greatest and quickest improvements in environmental protection by avoiding the generation of waste and harmful emissions. Source reduction makes the regulatory system more efficient by reducing the need for end-of-pipe environmental control by government. Adopting pollution prevention practices and techniques often benefits industry by lowering a company's operational and environmental compliance costs. By preventing the generation of waste, pollution prevention can also reduce or eliminate long-term liabilities and clean-up costs. Furthermore, disposal costs are reduced when the volume of the waste is decreased. This can also lead to a reduction in workplace exposures to hazardous materials which can affect the worker's health and hence their productivity.

PP-62

Re-Investigation and Synthesis of 2-Methyl Benzimidazole Derivatives

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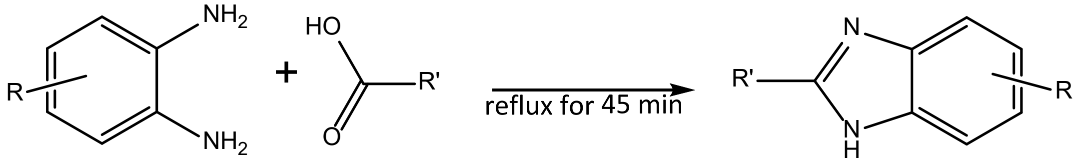
Benzimidazole a bicyclic aromatic compound (C7H6N2) consists of the fusion of benzene and imidazole ring. Benzimidazole, versatile N-containing heterocycles were synthesized and characterized by spectroscopic techniques such as FT-IR, 1H-NMR, 13C-NMR, EI-MS and also evaluated for specific radio pharmaceuticals and elemental analysis. Presence of Benzimidazole moiety in various drugs are used as Anti-inflammatory[1], Anti-cancerous[2], Anti-hypertensive[3], Anti-microbial[4], Anti-diabetic[5], etc agents. Synthesis of this derivatives involve intermolecular cyclization between ortho-phenylenediamine with acid derivatives[6]. Biological and Pharmacological importance of Benzimidazole derivatives inspired for the synthesis of new effective and precise drugs in medicinal field.

Keywords: Benzimidazole, Anti-inflammatory, Anti-diabetic, Anti-hypertensive, FT-IR, EI-MS



Scheme: Synthesis of 2-methyl benzimidazole

R=H, EDG,;R'=Alkyl, Aryl

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PP-63

Re-investigation of Electrophilic Substitution Reaction of Prochiral Ketone

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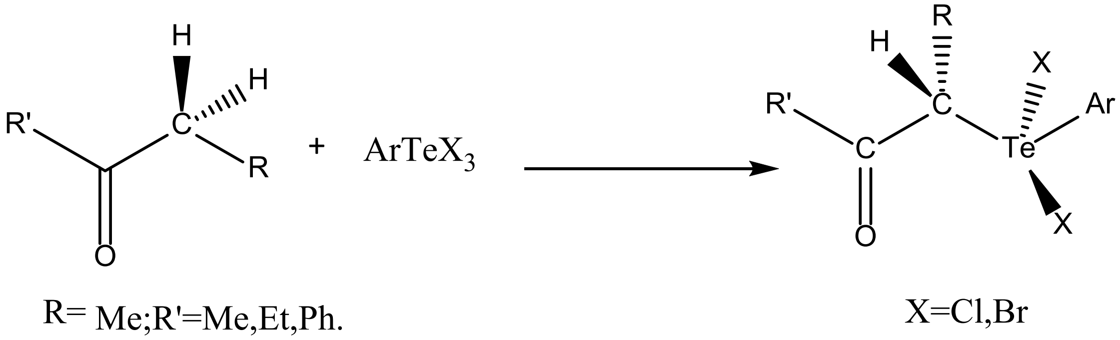
The direct interaction of aryltellurium trichalides, $ArTeX_3$ (Ar =1-naphthyl, A; mesityl, B; anisyl, C; X = Cl, a; Br, b)with Prochiral ketones, RCH_2COR'(R = Me, R’ = Ph, 1; Me,2;Et,R’ = Ph, 4), at room temperature gives mixed (acylmethyl/aryl) diorganotellurium dihalides where the acymethyl ligand bears an symmetric carbon[1] centre. The isomerically pure racemic mixture of aryldihalotellurated chiral ketone, $RCOC^*HMe(TeArX_2)$ have been isolated in good yield expect in the reaction between 1-naphthyltellurium trihalides and ethylmethyl ketone that affords a mixture of a-tellurated ketone with and without an asymmetric carbon. Aryltellurium reiiodides do not react. The isolated products have been characterized by C, H analyses, infrared, ^1H, ^{13}C, ^{125}Te NMR and mass spectral techniques. The central tellurium atom among the lattices of chiral compounds achieves six coordination via intermolecular Te…X/Te….O secondary bonding interaction while it remains five coordinate in the achiral compound.

Keywords: α-tellurated Ketone, Functionlized Organotellurium, Electrophilic Telluration, Secondary Bonding Interaction



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PP-64

Effectiveness of Carbohydrates in Life and Kinetic and Mechanistic Studies of the Oxidation of Fructose in Alkaline Medium

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Carbohydrates are vital to human survival and it is somewhat surprising that their study took so long to emerge a glamorous area of research. Carbohydrates serve as a structural material (cellulose), a component of the energy transport compound ATP, recognition sites on cell surfaces and one of three essential components of DNA and RNA. Carbohydrates including sugars are multifunctional naturally occurring material. An oxidation study of monosaccharide by different oxidizing agents is of special importance due to their biological relevance. Fructose has advantages for certain groups, including people with diabetes and those who are trying to control their weight. It is known as a simple sugar because it is single sweetening molecule. Fructose solution are employed to replace or supplement oral consumption of food or water in order to provide calories water in the body, to spare body proteins, to lower the production of excess ketones by liver. In the present study, the Ir(III)-catalysis of the iodate oxidation of fructose in aqueous alkaline medium has been investigated at 25°C The reactions exhibit first order kinetics with respect to lower $[IO_3^-]$ and $[OH^-]$ and show zero order kinetics at their higher concentrations. Unity order at low concentrations of fructose becomes zero order at its higher concentrations. The reaction rate is found to be directly proportional to [Ir(III)] in the oxidation of fructose. The mechanism consistent with kinetic studies, spectral evidences of reactive species and product analysis has been proposed for the oxidation of fructose in alkaline medium of iodate.

Keywords: Carbohydrates, Kinetics, Oxidizing Agent, Iridium (III), Fructose, Potassium Iodate

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PP-65

Importance of Carbohydrates in Nature and Mechanistic Studies of the Oxidation of Sucrose in Alkaline Medium

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The Study of carbohydrates is one of the most exciting fields of organic chemistry. Ubiquitous in the natural environment, carbohydrates perform important bodily functions. Among the most important are regulation of blood glucose and provision of energy for the body. In addition, carbohydrates spare the use of proteins for energy until the body is completely depleted of carbohydrate stores. They can be used as flavorings and sweeteners and are a source of dietary fiber. Sucrose a Disaccharide of Glucose and Fructose often found in all Photosynthetic Plants. Sucrose can be found in many medical dosage forms such as chewable tablets, syrups, lozenges or gums. Sugar derivatives have been shown to have therapeutic action in some condition. Sucralfate (aluminium salt of sucrose octasulphate) is used in treatment of peptic and stomach ulcers. Sucrose Polyesters have also been used as contrast agents in magnetic resonance imaging (MRI).In view of pharmaceutical and medical importance of sucrose, the kinetic oxidation of sucrose with iodate as an oxidant and Ir(III) chloride as an homogeneous catalyst in alkaline medium has been investigated. The reactions exhibit first-order kinetics with respect to lower [IO_3] and [OH] and show zero-order kinetics at their higher concentrations. Zero order kinetics in [sucrose] was observed throughout its variation. First order kinetics observed at lower concentration of [Ir(III)] in the oxidation of Sucrose. On the basis of kinetic orders, spectral information, a suitable scheme has been proposed for the oxidation of sucrose by iodate in alkaline medium.

Keywords: Mechanism, Sucrose, Potassium Iodate, Alkaline Medium, Ir(III) Catalyst

PP-66

Antiproliferative Potential of Novel 1,2,3-triazole based Artemisinin Derivatives

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Artemisinin is a sesqueterpene class of natural product isolated from the leaves of Artemisia annua plant. It is a sesqueterpene lactone endoperoxide having 1,2,4-trioxane system. Artemisinin derivatives are effectively used for the treatment of malaria. Anticancer potential of artemisinin has been first time reported by Woerdenbag et al. in 1993. After that many synthetic derivatives of artemisinin have been developed which showed significant anticancer activity. Since toxicity is the major concern for anticancer chemotherapy and artemisinin derivatives are generally found to be less toxic as compared to existing anticancer drugs. We have designed and synthesized two series of 1,2,3-triazole based derivatives of artemisinin and investigated their antiproliferative activity against different human cancer cell lines. Compound 9 showed potent antiproliferative activity against the A431 cell line (IC50=4.06 μM) and compound 17 displayed potent activity against the A549 cell line (IC50=7.16 μM). Further these compounds showed significant cell cycle arrest at G2/M phase and induce ROS production. An erythrocyte osmotic fragility assay study suggested the non-toxic nature of both the compounds 9 and 17 at a high concentration of 100 μg/mL. Mode of Presentation: Poster

PP-67

Sterically Hindered Organobismuth Compounds TRIS(α-Naphthyl) Bismuth(III) $(\alpha\text{-}C_{10}H_7)BiX_{3\text{-}n}(n=1,2)$ AND TRIS(Naphthyl) Bismuth (V) $(\alpha\text{-}C_{10}H_7)BiX_{5\text{-}n}$ (n=2,3,4) Derivatives

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A voluminous amount of work on organometallic compounds of bismuth both in +3 and +5 oxidation has been reported in the past few years but the work is mainly confined to the derivatives based hydrocarbon residue like phenyl, methyl haloalkyl ($-CF_3$),halophenyl ($-C_6F_5$) etc. bonded to meta atom and only limited work has been reported on compounds having sterically hindered naphthyl, Cyclohexyl or mesityl groups. The introduction of the latter groups render hydrolytic and thermal stability compared to phenyl based analogues [1-20]. The nature and chemical behavior of bismuth compounds issomewhate different from antimony and arsenic. For example the oxidative reactions with electrophilic reagents like $(SCN)_2$ is preferred with triarylantimony and triarylarsenic compounds but in case of bismuth compounds cleavage of organic group is preferred over cleavage reaction.

$$Ar_3Sb + (SCN)_2 \longrightarrow Ar_3Sb(NCS)_2 \quad \cdots\cdots\cdots(1)$$

$$Ar_3Bi + (SCN)_2 \longrightarrow Ar_2BiNCS + ArSCN \quad \cdots\cdots\cdots(2)$$

However in case of bulky groups stability of cyclohexyl or naphthyl group bonded to arsenic, antimony and bismuth compounds is more pronounced over the other organic derivatives of these metals.

A perusal of literature reveals that cyclohexyl and naphthyl based compounds of arsenic and antimony have been studied to a considerable extent but the information on organobismuth compounds is trivial. The synthesis of tris (α- naphthyl) bismuth was reported by challenger in 1914 [21] along with $(\alpha\text{-naphthyl})_3BiCl_2$ $(\alpha\text{-naphthyl})_2BiCl$ and $(\alpha\text{-naphthyl})_3BiBr_2$. Since then some work on imides, amides and carboxylates has been done particularly by our research but the chemical behavior of $(\alpha\text{- naphthyl})_3$Biand its derivatives is yet to be studied.

Thus the object of the present work was two fold (i) oxidative addition or cleavage reaction of tris(α- naphthyl) bismuth(III) employing halogens, pseudohologens and inter halogens and Metallic halides (ii) To examine the stability of naphthyl based derivatives of bismuth vis-à-vis phenyl derivatives along with their biological activity.

The paucity of the published data on sterically larger organobismuth compounds with α- naphthyl moieties encouraged us to undertake a systematic study on the

1. Synthesis and isolation of four different types of bismuth(III) halides and bismuth (V) halides having varying content of bulky α- naphthyl groups,$R_nBiX_{3\text{-}n}$,$(\alpha\text{-}C_{10}H_7)BiCl_2$ reported earlier has also been obtained through redistribution reaction.
2. Synthesis and isolation of α- naphthyl bismuth (V) dichloride $R_nSbCl_{5\text{-}n}$ (n=1,2) and mixed halides $RBiCl_2Br_2$.

3. Mixed halo carboxylates of the formula (α-$C_{10}H_7$)BiClL and (α-$C_{10}H_7$)BiLL'(L=monocarboxylates; L'=dicarboxylates) and (α-$C_{10}H_7$)BiL_2.
4. Synthesis of halo-imides of the type (α-$C_{10}H_7$)BiClL
5. Synthesis of halo oximates (α-$C_{10}H_7$)BiClL

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PP-68

Synthesis and Evaluation of Antioxidant Activity of Pyrrole-Based Imidazole Chalcones: Experimental and DFT Study

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Heterocycles are very important functional groups, especially in medicinal chemistry. They are not only pivotal in the synthesis of drugs, but also form part of the structure of a diversity of drugs, vitamins, natural products and biomolecules. The importance of imidazoles in heterocycles lies in the fact that their derivatives are known for analgesic, antifungal, antihypertensive, antiobesity, anticancer and other biological activity. Additionally, they can inhibit butyrylcholinesterase, acetylcholinesterase, carboxylesterase and quorum sensing. Chalcone, an important intermediate of flavonoid synthetic pathway, has been shown to exhibit diverse biological and pharmacological activities such as anti- cancer, antioxidant, anti-inflammatory, etc. In this study, a novel series of pyrrole imidazole chalcones have been synthesized by neat reaction method. The structures of all compounds are confirmed via a wide range of spectroscopic techniques including IR, 1H and 13C NMR and mass spectra. Significantly, all synthesized compounds have been tested for their promising antioxidant activities via utilization of 1,1-biphenyl-2-picrylhydrazyl as a free radical scavenging reagent. Surprisingly, the results demonstrated that synthesized compounds good antioxidant activity. Furthermore, the role and contribution of different functional groups on the antioxidant activity of the synthesized chalcone derivatives are also probed and rationalized in terms of their electronic and structural effect.

Keywords: Pyrrole, Chalcones, Antioxidant Activity, Pharmacological Activities

PP-69

Environmental Friendly Synthesis, Structural Elucidation and Evaluation of NLO Properties of Dipyrromethane Derivatives

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Green chemistry is defined as the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances. For the purposes of this definition, synthetic chemists have great interest in developing highly efficient transformations for the preparation of organic compounds. One of the main themes of contemporary synthetic organic chemistry is the use of environmentally feasible reagents particularly in solvent-free conditions and environmentally benign catalytic systems, which are also required to be efficient and economic. Solvent-free organic reactions are usually rapid, eco-friendly, high yielding and economically viable. In this context, organic reactions under solvent-free conditions at room temperature have been achieved. Dipyrromethanes are compounds known for more than a century and are widely being used as important building blocks for the synthesis of porphyrins, Calixpyrrols and Corroles. In particular, the interest to these compound are being due to the various applications in the biological, material and coordination chemistry and fact that the pyrrole is in many natural pyrrole assemblies. This study describes a successful approach for the synthesis of dipyrromethanes using iodine as a catalyst on grinding. This protocol does not require any solvent and carried out at lowest pyrrole/aldehyde ratio which makes this method economically and environmentally attractive. This protocol affords the products immediately with excellent yield. The molecular structure and detailed spectroscopic analysis of a novel synthesized dipyrromethanes have been performed using both experimental techniques (^{1}H NMR, UV–Visible, FT–IR and Mass) and theoretical calculations. Natural bond orbitals (NBO$_s$) analysis has been carried out to investigate the intramolecular conjugative and hyperconjugative interactions within molecule and their second order stabilization energy ($E^{(2)}$). TD–DFT has been used to calculate oscillatory strength (f) and wavelength absorption maxima (λ_{max}) of various electronic excitations and their nature within molecule. To investigate the strength and nature of H–bonding, topological parameters at bond critical points (BCP) have been analyzed by 'Quantum theory of Atoms in molecules' (QTAIM). Local reactivity descriptors as Fukui functions (f_k^+, f_k^-), local softnesses (s_k^+, s_k^-) and electrophilicity indices (ω_k^+, ω_k^-) analyses are performed to find out the reactive sites within molecule. The chemical shift for *meso*–proton of all studied compounds has been observed in the range of 5.54-5.55 ppm as singlet confirms the formation of dipyrromethane molecules. The first hyperpolarizability (β_0) has been computed to evaluate the non–linear optical (NLO) response of the investigated molecule. The first hyperpolarizability of all studied compounds has been found in the range of 6.55-20.88 x10^{-30} esu indicating their possible use for NLO applications.

Keywords: Dipyrromethane, Hydrogen–bonding, QTAIM, First Hyperpolarizability

PP-70

Synthesis and Spectroscopic Study of Antitubercular Pyrrole-pyridine Hydrazide-Hydrazone

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The unusual structure and chemical composition of the mycobacterial cell wall, the tedious duration of therapy and resistance developed by the microorganism have made the recurrence of the disease multidrug resistance and extensive or extreme drug resistance. The need to synthesize new drugs that will shorten the total duration of effective treatment and/or significantly reduce the dosage taken under DOTS supervision, improve on the treatment of multidrug-resistant tuberculosis which defies the treatment with isoniazid and rifampicin and provide effective treatment for latent TB infections which is essential for eliminating tuberculosis prompted this review. In the present investigation, pyrrole pyridine hydrazide-hydrazone derivative have been synthesized in good yields and structures of these compounds were established by IR, ^{1}H NMR, ^{13}C NMR, mass spectral and elemental analysis. The newly synthesized title compounds were evaluated for their antimicrobial as well as antimycobacterial activities. The tested compound displayed promising anti-tubercular activity. The result revealed that this compound exhibit anti-tubercular activity at non-cytotoxic concentrations.

Keywords: Multidrug, Pyrrole Pyridine, Hydrazide-Hydrazone, Antimycobacterial

PP-71

Triphynylantimony(V) Carboxylates and Cycloantimonates; Biological Perspective, Screening & Assessment of Cyclotoxic, Antifungal and Antitumour Activity

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The synthesis and characterization of a number of triphynylantimony derivatives has been reported. In several cases structural conclusions have been derived with the aid of spectroscopic evidences and X-ray crystallography. These studies were mainly involved to solve the problem of trigonal-bipyramidal (TBP) or square-pyramidal (SP) geometry which has been frequently established in case of phosphorus. The preferred geometry of Group 15 elements is a TBP which is fluxional, stereochemically non-rigid or pseudorotating arrangement rapidly interconverting with the alternative square-pyramidal structure. The energy different between the two structural alternative is small both in solution and in the solid state where the nature of the counterion for charged species lattice effects and the solvent of crystallization play a determining role. In this way, delicate balance exists between the TBP and SP forms, both in solution and the solid state. An appreciation of the pseudorotation processes occurring the life time of a five coordinate intermediate is clearly important for predicting and ultimately controlling product stereochemically.

The main concern of the investigation has been with the stereochemically of the pentavalent antimony derivatives and the biological aspects have seldom been looked into. Though in a number of cases organoantimony(V) derivatives along with organoantimony(III) derivatives have shown remarkable antimicrobial and antitumour activity.

The present investigation on organoantimony(V) carboxylates and cyclometallates was under taken with a view:

- To investigate chemical behavior as well as constitution of organoantimony(V) carboxylates, linear or polymeric and change in the nature of organoantimony(V) carboxylates on changing the carboxylic group.
- To isolate hitherto unreported organoantimony(V) carboxylates.
- To investigate the biocidal and antitumour activity associates with organoantimony(V)-carboxylates and-cyclometallates.

Since one of the major aims of presents investigation was focused on the biological activity of organoantimony compounds, the author synthesized a series of triphenylantimony(V) derivatives with salicylic acid, benzillic acid, mandelic acid and its derivatives, aspartic acid, 2-pyrazine carboxylic acid and naproxene. The structure of few compounds is well established by X-ray differaction method and therefore in turn helped to established structure activity relationship.

PP-72

Triphynylantimony(V) Carboxylates and Cycloantimonates; Biological Perspective, Screening & Assessment of Cyclotoxic, Antifungal and Antitumour Activity

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The synthesis and characterization of a number of triphynylantimony derivatives has been reported. In several cases structural conclusions have been derived with the aid of spectroscopic evidences and X-ray crystallography. These studies were mainly involved to solve the problem of trigonal-bipyramidal (TBP) or square-pyramidal (SP) geometry which has been frequently established in case of phosphorus. The preferred geometry of Group 15 elements is a TBP which is fluxional, stereochemically non-rigid or pseudorotating arrangement rapidly interconverting with the alternative square-pyramidal structure. The energy different between the two structural alternative is small both in solution and in the solid state where the nature of the counterion for charged species lattice effects and the solvent of crystallization play a determining role. In this way, delicate balance exists between the TBP and SP forms, both in solution and the solid state. An appreciation of the pseudorotation processes occurring the life time of a five coordinate intermediate is clearly important for predicting and ultimately controlling product stereochemically.

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PP-73

Impacts of Environmental Air Pollution on Human Health

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Abstract

In this present study Examined to control the pollutants coming from different industries. To maintain the environmental sustainability by controlling the pollutants. All living organisms damage caused by pollution. This is coming from most of chemical industries. It is an unwanted impact in the physical, chemical and biological characteristics of air, water and soil that may harmfully affect the human life and it creates a potential health hazard of any living organism. Industrialized countries of the world such as United states of America, India ,Germany, Japan, Dubai, Nigeria, Saudi Arebia, China, Texas released Nox ,SO2 gas, pesticides, detergents, plastics, solvents, fuels, paints, dyes, food additives,CO,CO2in to environment. These are very hazardous to human being as well as plants and animals. There are a number of industrial effluents emissions of poisonous gases in to the atmosphere. Mining activities also added to this problem, particularly as solid waste. The unsafe conditions created by man himself and cause to unsustainable of environment. The man made activity leads to damage not only human survival nature but also all other living organisms.

PP-74

Photovoltaic Panel: Environmental Impacts of Renewable Energy Technologies

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Nowadays, fossil fuels are the main sources of energy from which electricity is obtained. But these sources will not last forever, so in due course renewable energies will have to replace them in this role. All energy sources have some impact on our environment. Fossil fuels oil, and natural gas do substantially more harmful than renewable energy sources by most measures, including air and water pollution, damage to public health, wildlife and habitat loss, water use, land use, and global warming emissions. Photovoltaic's is now a proven technology which is inherently safe, as opposed to some dangerous electricity generating technologies. Over its estimated life a photovoltaic module will produce much more electricity than was used in its production. A 100 W module will prevent the emission of over two tonnes of CO_2. Photovoltaic systems make no noise and

cause no pollution while in operation. Photovoltaic panel technologies that have relatively lower environmental risks compared to other types of electric sources. However, chemicals used in PV cells could be released to air, surface water, and groundwater in the manufacturing facility, the installation site, and the disposal or recycling facility. This paper focuses on utilization of renewable energy devices as photovoltaic cell and emphasize the various applications and methods to promote the benefits of solar energy production and its potential for reducing environmental pollution that ensure overall sustainable development in India.

Keywords: Renewable energy, Solar panel, Photovoltaic cell, PV Panel, Solar Concrete Collecto

PP-75

Boron Decorated Graphene as H2S Sensor: DFT Study

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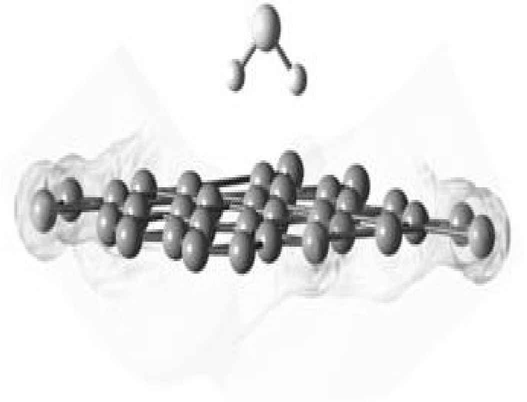
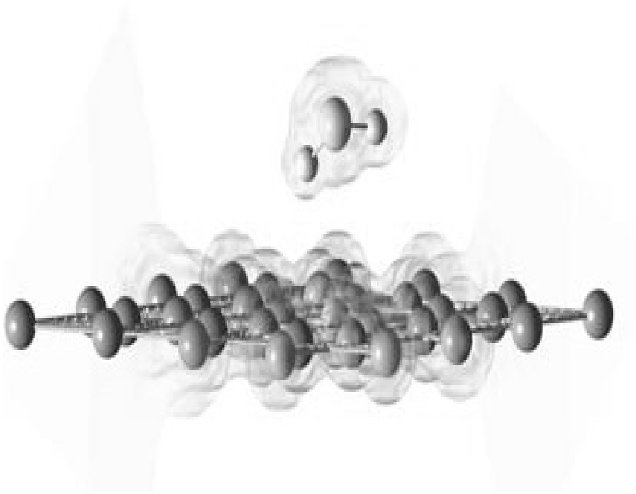
The adsorption of toxic H2S on the surface of pristine as well as boron decorated graphene are investigated using density functional theory based ab-initio approach, applied through Generalized Gradient Approximation with Perdew, Burke and Ernzerhof type parameterization. Since boron has one odd electron showing two spin (α and β), the most stable geometry of H2S gas molecule on pristine and Boron decorated graphene are determined through Homo-Lumo gap as with β spin and the adsorption energies are calculated. The computed adsoption energy of H2S absorbed pristine and Boron doped graphene sheet confirms relatively weak physisorption in case of pristine graphene. Further the adsorption of H2S gas on pristine and boron decorated graphene sheet has been analysed through Bandstructure, density of state and Electrostatic potential (ESP). On adsorption of H2S gas on the surface of pristine graphene does not show any significant change in bandgap, however in case of B-doped graphene, the band crossing and conductance variation confirms the H2S sensing.





PP-76

Green Synthesis of Metal Nanoparticle using Enzyme

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Green synthesis of metal nanoparticles(NPs) using enzyme has been an important area of research owing. Application of nanoparticle in many fields including diagnostics, catalysis, optics, medical and therapeutics. Metal based nanoparticles have gain wonderful popularity because of their interesting physical, magnetic, biological and optical properties. Extracellular and intracellular enzymes are play a important role in synthesis of nanoparticles. In this review it is reported that the biosynthesis of nanoparticles using enzyme like α-amylase, laccase, lignin, trypsine, cellulose reductase. The synthetic nanoparticles like Gold nanoparticle (AuNPs), Silver nanoparticle (AgNPs). Enzymes are widely used in many industrial and pharmaceutical areas due to their capacity to catalyze reactions with high selectivity. In most cases, multiple enzymes will be contained within a single nanoparticle or medium, but in recent years researchers to cover up individual enzymes within single enzyme nanoparticles (SENs). Integration of the principles of green chemistry with nanotechnology has been play important role in nanoscience and has received great attention in latest years. Biological methods are used for the green synthesis of metal and metal oxide nanoparticle of desirable size and morphology and they develop the properties of nanoparticles in greener route.

PP-77

Synthesis and Characterization of ZTO Nanoparticles using Green Sol gel Method

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Nanosize zinc tin oxide nanoparticle has been synthesized by green sol gel method using extract of Aloe Vera and Cauliflower. The synthesized sample was characterized by using Scanning Electron Microscopy (SEM), EDX, UV visible spectroscopy and FTIR spectroscopy. Green synthesized ZTO nanoparticles were found to be stable having various attractive properties with low cost of preparation and low toxicity as compared to other conventional physical and chemical synthesis methods. The optical band gap of synthesized nanomaterial was found to be 3.37 eV. The average particle size of the ZTO was calculated by using particle size analyzer and found to be 120 nm. EDX data confirms the formation of zinc tin oxide nanoparticle. These nanoparticles have very high surface reactivity so it can be used in so many applications.

Keywords: Green synthesis, Sol-Gel, SEM, EDX

PP-78

Contemporary Aspects in the Sustainable Synthesis of Quinazolinone and its Derivatives Utilizing Isatoic Anhydride

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Quinazolinone and their derivatives are the nitrogen containing heterocyclic moiety that are considered as a fascinating chemical compound due to their broad-spectrum physiological significance and pharmacological utility. They reveal various medicinal properties namely anti-inflammatory, anti-microbial, antifungal, antibacterial, anticancer, immunotropic, antiulcer and analgesics. These heterocyclic compounds are valuable intermediates in organic synthesis and are synthesized efficiently via one-pot three-component strategy involving condensation of isatoic anhydride as a main substrate with differently substituted aldehyde and amine. The above reaction methodology involves green solvents and green catalysts thus approaching towards a safer, energy efficient and less hazardous synthesis. The implementation of the twelve principles of green chemistry in the synthesis of quinazolinones is a relatively new emerging affair concerning the sustainability.

Keywords: Quinazolinone, Isatoic Anhydride, Green Synthesis.

PP-79

Modified Polyol-mediated Synthesis of Orthorhombic Zirconia from bis Cyclopentadienyl Zirconium (IV) di-chloride in Presence of Argon gas.

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ABSTRACT

Zirconium oxide (ZrO_2) nanoparticles have been successfully synthesized by using bis cyclopentadienyl zirconium (IV) di-chloride using argon gas atmosphere for the first time. Synthesized ZrO_2 nanoparticles were calcinated at 500° C under air atmosphere and characterized using X-ray powder diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, EDX, scanning electron microscopy (SEM) and Transmission Electron Microscopy (TEM) for their formation, structure, morphology, size, and elemental composition. XRD results revealed the formation of monoclinic and orthorhombic polymorph of ZrO_2. The single crystallite size was obtained using Scherrer formula which is in the order of 1.7 nm from most intense XRD peak. The strong FTIR absorption peak at 470.54 cm -1 region confirmed the formation of ZrO 2 structure. EDX spectrum confirmed that Zr and O elements are present almost in stiochoimetric ratio. SEM and TEM images of ZrO 2 demonstrated fine and uniform particles in nanometer range.

Keyword: Zirconia (ZrO 2), Orthorhombic Zirconia, Polyol Synthesis, Crystal Structure

PP-80

Green and Dynamic Contribution of Plant Growth Promoting Rhizobacteria for the Sustainable Agriculture Development

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ABSTRACT

Chemical fertilizers and pesticides are used to enhance the growth and production of agricultural crops since many years. Although, these chemicals increase the crop yield, but also affect the soil micro flora and fauna and cause several health hazards including human. In addition, it also distresses the fertility and biodiversity of the soil and effects on the ecosystem. To overcome this problem, an economically attractive and eco-friendly technique of using beneficial plant growth promoting rhizobacteria (PGPR) are increasing day by day. The use of plant growth promoting rhizobacteria are better option for enhancement and productivity of crops by the colonization of roots. PGPR enhance the growth and yield directly such as production of indole-3 acetic acid, siderophore, solubilization of phosphate, zinc and potassium and indirectly by growth inhibition of phytopathogens associated with host plant. Thus, the use of PGPR in the agricultural crops could be an excellent strategy to growth, and yields of agricultural crops as well as reduction of chemical fertilizers and pesticides and for the sustainable agricultural development.When we study the several research papers about the role of plant growth promoting rhizobacteria in sustainable agriculture. We will discuss about the direct and indirect mechanism of PGPR.

Keywords: Bio-fertilizer, Bio-pesticide, Plant Growth Promoting Rhizobacteria, Sustainable Agriculture

Full Research Paper (FRP)

FRP-01

Adsorption and Conformation of Carboxymethyl Cellulose at TiO_2-Modified Mesoporous Carbon Derived from Mustard Cake

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Abstract—Our knowledge and understanding of the binding mechanism of carboxymethyl cellulose (CMC) onto solid-liquid interface continuous to improve year by year. However, previous work indicates that there is no consensus among authors on its binding mechanism. An attempt has, therefore, been made on binding aspects of CMC onto TiO_2- modified mesoporous carbon derived from mustard cake employing SEM, ATR FTIR, XRD, BET, AFM, XPS and other allied spectroscopic techniques. The adsorption of the CMC onto TiO_2-modified carbon derived from mustard cake was found to be influenced markedly by a change in solution conditions and confirmed by ATR FTIR, fluorescence spectroscopy, and other techniques. The adsorption free energy of CMC was found as ~ -22 kJ/mol which was in close agreement with H-bond energy suggesting hydrogen bonding to be a dominant force for CMC L2 type adsorption (in the present study). The presence of urea decreased the adsorption of CMC, considerably which added assurance that adsorption in the present case is attributed to the presence of hydrogen bonding. XPS and ATR FTIR also support that electrostatic interaction and hydrogen bonding is responsible for adsorption of CMC onto TiO_2-modified carbon surface. Fluorescence spectroscopy study demonstrates that there's no evidence of the formation of hydrophobic domains onto TiO_2-modified carbon/water interface in acidic medium. All of the above results coupled with reported facts suggest that the adsorption of CMC onto the TiO_2- modified carbon derived from mustard cake is a complex interplay of electrostatic attraction, hydrogen bonding and hydrophobic force depending on the experimental conditions.

Keywords CMC adsorption; Carbon; ATR FTIR; BET; AFM; XPS.

INTRODUCTION

Carboxymethyl cellulose (CMC) is a natural anionic polysaccharide which is water-soluble, non-toxic and biodegradable in nature. The CMC has industrial applications in food industry under the trade name of E. No. 466 as viscosity modifier, thickener and to stabilize emulsion in various products including ice cream. It is also used in non-food products such as toothpastes, detergents, sizing and coating compositions in pulp impregnants in paper and textile industry. It is also used as lubricant in artificial tears as a thickening agent in the oil drilling industry as an ingredient of drilling mud. It is sometime used an electrode binder in advanced battery application especially with the graphite anode (Hollabaugh et al. 1945). The CMC is extensively used as depressant, dispersant as well as flocculants in mineral processing especially in the flotation of sulfides ores (Tian et al. 1984). The most important industrial and analytical derivative of the CMC is its sodium salt (cellulose gum) (Rhodes 1979; Steenberg and Harris 1984; Jin et al. 1984). There are several repeating units in the structure of CMC (Fig. 1) in which three $^-$OH groups present on each unit of CMC are responsible for H-bonding (Mackenzie 1980). Our understanding to binding mechanism of the CMC at solid-liquid interface has been increasing year by year as significant work has been devoted to adsorption of CMC onto the mineral surfaces. Several binding mechanisms have been developed, but as yet no common mechanism has received general acceptance. Thus, the associated problems have received adequate attention. Raju et al (1987) reported the adsorption of polysaccharides (dextrin) onto graphite is apparently due to hydrophobic-hydrophobic interaction. Laskowski's investigation on adsorption of CMC on graphite has shown that while pure high-quality graphite (Ceylon) adsorbs CMC strongly. However, the same graphite purified by leaching practically does not adsorb CMC almost at all (Solari et al.1986). Mackenzie et al (1986), Pugh (1989), Healy and Macromol (1974) and Rath et al. (1997) proposed adsorption of CMC at mineral water surfaces is due to complex interplay of electrostatic, hydrophobic, hydrogen bonding and chemical interactions, although, the selective adsorption of CMC on minerals has not been demonstrated clearly. The binding mechanism of CMC on minerals was also proposed by Steenberg et al (1982,1984) and Jenkins et al (1998) and according to them adsorption occurs mainly at the basal planes via hydrophobic force. Contrary to this, Rath et al. (1995) and Jucker et al. (1997) proposed the binding mechanism of polysaccharides attributing to hydrogen bonding on solids. Based on infrared spectroscopy Bakinov et al. (1964) reported some changes in the carboxyl group upon adsorption and suggested that the carboxyl group interacts with metal ions on the surface of soild (talc). However, the infrared spectra were recorded using a transmission with dried samples causing any deduction on polymer binding mechanisms to be overshadowed by the substantial alteration to the polymer's environment during dehydration. Furthermore, no infrared spectra were actually presented in this work. Wang and Somasundaran (2005) also used infrared spectroscopy to support their hypothesis of hydrogen bonding; however, their work also involved sample drying and analysis by infrared transmission. Cuba-Chiem et al. (2008) on the basis of in situ film ATR FTIR spectroscopy (in liquid form) has proposed that the polymer (CMC) most likely has two different interactions with the solid surface, with a stronger interaction with the talc edge through chemical complexation and a weaker interaction with the talk basal plane presumably through the hydrophobic interaction. Fujimoto and Petri (2001) also studied adsorption behavior of CMC on amino-terminated surfaces and reported that CMC adsorbs onto amino-terminated surfaces driven by electrostatic interactions. The adsorbed amount decreases with ionic strength, in agreement with the screening-reduced adsorption regime. The charge on the amino-terminated substrate and segment charge along the CMC chains is strongly influenced by the pH. However, the adsorption behavior is mainly controlled by the surface charge. The above literature clearly illustrates that there is lack of consensus among various investigators for the binding mechanism of CMC onto the solid-liquid surface.

None of the previous work on CMC adsorption on solid/water interface has involved in-depth characterization such as surface charge on adsorbent, BET, urea test, ATR FTIR spectroscopy (in solid form) and XPS. The objective of this study, therefore, is to clarify and to substantiate the mechanistic aspects of the interactions between CMC and solid surface (TiO_2-carbonized carbon in the present case) employing in-depth characterization using various techniques.

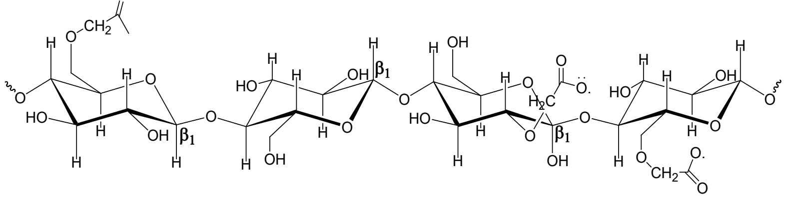


Fig. 1 The monomeric structure of CMC

EXPERIMENTAL

MATERIALS

CMC was purchased from Akshar Exim Company Private Limited Kolkata. The mustard cake (MC) sample collected from the mill was crushed and washed with distilled water and then sun-dried. This material was treated with 20 wt% H_2O_2 at 60°C for 24 h to oxidize the adhering organic matter and it was washed several times using double distilled water. This powder was burned in the presence of N_2 gas at 715°C for 25 min. The material, powdered activated mustard carbon (PAMC) was grounded and sieved to desired particle sizes. To get TiO_2-modified carbon, TiO_2-Degussa P25 (ca.80% anatase, 20% rutile) was added to PAMC in a 5:1 weight ratio, in NaOH 2N alkaline solution; in the 1000 ml volumetric flask with reflux condenser, the new adsorbent (TiO_2-modified carbon) was obtained from the slurry under stirring (300 ppm) for 24h, at atmospheric pressure and 100^0C, on a thermostat heating plate. After filtration, washing and drying at 105-120^0C till constant mass, the dried TiO_2-modified carbon was ground and passed through a100 mesh sieve and stored in a desiccator. The TiO_2-modified carbon was further used in experiments for adsorption and conformation of carboxymethyl cellulose.

The morphological studies of the PAMC and TiO_2-modified carbon were done using scanning electron microscope (SEM) analysis. Mica in the form of flat plate was also used in AFM studies. A stock solution was prepared by quickly adding 0.23 g of CMC powder into 500 ml of vigorously stirred distilled water and further stirring for 30 min. The solution was then refrigerated overnight to complete hydration of CMC and any undissolved impurities were removed by filtration (Whatman#4).

In the experimental studies, the pH of the solutions was mentioned and adjusted at the desired values using standard NaOH and HCl. In the fluorescence studies, the probe labeling of the polymer was done by using double distilled water. Urea (Fischer Chemical), phenol (Aldrich) and 98% sulphuric acid (Fischer Chemical) were used for the colorimetric experiments. Solutions were prepared in the double distilled water.

METHODS

ADSORPTION MEASUREMENTS

The solutions were prepared using stock solution for adsorption measurements. In a known solution of CMC, TiO_2-modified carbon (0.50 g) was loaded and left for conditioning overnight. The residual concentration CMC was determined after centrifugation of suspension employing UV spectroscopy (λ_{max} = 265nm). The adsorption density of CMC on TiO_2-modified carbon was calculated using following equation:-

$$qe = \frac{(Co - Ce)V}{m}$$

Where C_o and C_e are initial and equilibrium concentrations (mg l^{-1}) of CMC in the solution, V the volume (l), m the weight TiO_2-modified carbon and q_e is the amount of CMC adsorbed by the TiO_2-modified carbon (mg g^{-1}).

ELECTROKINETICS MEASUREMENTS

The surface potential of TiO_2-modified carbon may be influenced by the pH value of the coexisting liquid bulk phase. The pH value, at which the surface charge is zero, is called the point of zero charge (PZC). The surface is positively charged at $pH < pH_{PZC}$ and negatively charged at $pH > pH_{PZC}$.

SEM ANALYSIS

The particle morphologies of the TiO_2-modified carbon was investigated employing Scanning Electron Microscope of JEOL (JSM 6490LV).Prior to SEM analysis mounted samples were coated with gold palladium.

ATR FTIR Spectroscopy

Vibrational spectroscopy in the infrared region was used to perform the characterization of the molecular structure of the adsorbent from the vibrational modes related to functional groups present in the adsorbent. The ATR FTIR spectra were obtained using an attenuated total reflection fourier transformation infra-red (ATR FTIR) Bruker *Tensor 27* and OPUS data collection program.

X-ray diffraction study

Crystallographic parameters of the TiO_2 modified activated carbon were obtained from X-ray diffraction (XRD) studies. Powder X-ray diffraction ($_p$XRD) patterns were recorded on a Rigaku Miniflex II desktop X-ray diffractometer at 30kV and using CuK radiation.

BET surface area measurements

The surface analysis, size and pore volume of the materials was performed using a surface area analyzer (BELSORP-max, Japan). A definite amount of the adsorbent materials (0.24 g) were heated at 400^{0}C under vacuum for approximate 5-6 hrs. Subsequently, the process of N_2 adsorption and desorption was performed. The surface area and pore volume were calculated using the standard Brunauer-Emmett-Tiller (BET) equation and pore size was obtained employing a method of Barrett-Joyner-Halenda (BJH).

Fluorescence Spectroscopy

The microstructure of the adsorbed layer was investigated by fluorescence spectroscopy which is essential for clear understanding the binding mechanism of CMC adsorption onto the carbonized mustard cake. Fluorescence spectroscopy is a well-developed method to investigate the existence the hydrophobic domain formation due to adsorption.

AFM Analysis

The atomic force microscopy (Agilent 5500) measurements were conducted in air and underwater in tapping mode using a V-shaped cantilever (Si_3N_4). This cantilever was covered with gold on the back for laser beam reflection. NP-20 AFM probe was used in air and underwater medium.

X-ray Photoelectron Spectroscopy Measurements

The XPS experiments were performed in an ultrahigh vacuum (UHV) using high-resolution X-ray photoelectron spectrophotometer (HR-XPS), PHI 5000 Versa Prob II, FEI Inc (1,486.6 eV; 100W; spot size, 10mm to 200 mm). All samples were dehydrated under vacuum prior to XPS analysis. The dehydrated samples were then lightly pressed onto individual pieces of tin foil using a hydraulic ram press. The prepared specimens were then attached on flat electron spectroscopy for chemical analysis (ESCA) stubs. The analysis stub was inserted into the fast entry chamber of the ESCA apparatus, where the pressure was reduced to about 1×10^{-6} Torr. The stub was then transferred into the analysis chamber of the ESCA apparatus, where the background pressure was of the order of 1.5×10^{-9} Torr. The surfaces of the pressed TiO_2 samples were scrapped in situ to expose fresh powder surfaces. Both survey and narrow region scans of C 1s and Ti 2p were conducted at 187.85 eV. All spectra were taken at polar angle 45^0. All data were background subtracted, smoothed using a five-point quadratic Savitzky–Golay algorithm, and charge corrected soals that the carbon-carbon bond had a binding energy of 285.0 eV. Data were plotted using Casa XPS Version 2.3.17PRI.I and Origin Pro 8 SRO v8.0724 (B724) software.

RESULTS AND DISCUSSION

Adsorption Studies

Effect of Concentration

Fig. S1 clearly illustrates the effect of concentration on adsorption isotherms of CMC on TiO_2-modified carbon which gradually increases as the concentration of CMC increases.

Effect of pH

Adsorption isotherm of CMC onto TiO_2-modified carbon at different pH was recorded (Fig. 2). It was found that the adsorption of CMC onto TiO_2-modified carbon surface at pH 3.0 was more in compression at pH 9.8. Since it was seen that the adsorption density of CMC was reduced significantly with increase in pH value from 3.0 to 12.0 (Fig. not shown). Thus, it can be concluded that electrostatic repulsion plays an important role in this system.

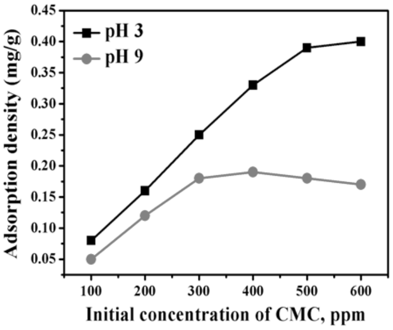


Fig. 2 Adsorption isotherms of CMC onto TiO_2-modified carbon surface at different pH values

Effect of Ionic Strength

Adsorption of CMC on TiO_2-modified carbon was studied by using solutions of different ionic strengths (Fig. S2). The amount of adsorption increases with the increase of ionic strength; this is because of screening effect of KCl. Therefore, at pH 9.8 the CMC and TiO_2-modified carbon are negatively charged, the addition of salt will reduce the electrostatic repulsion between them, resulting in an increase in CMC adsorption density.

Adsorption on TiO_2-modified Carbon (with and without urea)

To provide the experimental proof to show that hydrogen bonding plays a vital role in any adsorption process, experiments could be conducted in the presence of hydrogen acceptors/breakers such as DMSO and urea. In the present case, experiments were conducted by adding urea (0.1M) in adsorbate solution. Since, urea is a hydrogen bond breaker and if amount of adsorption decreases significantly, it provides substantial proof that occurrence of adsorption is attributed to hydrogen bonding. The results consisting with this statement were found in the present case and Fig. S3 clearly illustrates that adsorption tests using urea as solvent accompanied by significant reduction in amount of adsorption. Therefore, it is beyond doubt that the hydrogen bonding plays an important role in the present adsorbate-adsobent system. Similar results have been reported by other researchers for adsorption of CMC at talc/water interface (Wang and Somasundaran, 2005) and mechanism of adsorption of starch onto hematite (Weissenborm et al, 2995).

Modeling of CMC Adsorption on TiO_2-modified Carbon

To obtain a better understanding of the binding mechanism of CMC on solids, the standard free energy of adsorption (G^0_{ads}), the maximum amount of polymer adsorbed per mass of solid ($(x/m)_{max}$) and the effective surface area occupied per CMC chain (σ^0) at the TiO_2-modified carbon/solution interface was evaluated from adsorption isotherm(Table S1). The adsorption isotherm of CMC on TiO_2-modified carbon shows a pseudo-Langmuir adsorption isotherm. The Langmuir equilibrium isotherm (Singh et al. 2016) is based on the fact that the adsorption occurs at a specific homogenous site within the surface of adsorbent and monolayer sorption onto a surface with a finite number of identical sites assuming that there are no interactions between adsorbed molecules on the surface. Hence, covered surface by the polymer (CMC) is given by:

$$q_e = \frac{q_m K_L C_e}{1 + K_L q_m}$$

This can be linearized as,

$$\frac{C_e}{q_e} = \frac{1}{K_L\, C_e} + \frac{C_e}{q_m} \tag{1}$$

Where q_e(mg/g) is the amount of solute adsorbed per unit weight of adsorbent, C_e(ppm) is the equilibrium concentration of solute, q_m is the monolayer adsorption capacity (mg/g) and is a constant, and K_L is a constant related to the free energy of sorption ($K_L \alpha\ e{-}\Delta G/RT$). It is the reciprocal of the concentration at which the adsorbent is half-saturated. Values of the constants were evaluated using a plot of C_e/q_e vs. C_e (Fig. 3).

It is obvious that determination of equilibrium constant is a key towards correct estimates of $\Delta G^0_{ads}$where as the equilibrium constant for adsorption is related to the isotherm equation employed. In the sense of reaction thermodynamics, ΔG^0_{ads} can be evaluated according to the unitless thermodynamic equilibrium constant whereas Langmuir equilibrium constant has a unit of lm^{-1}. The parameter K_L from the Langmuir formula can be used as K_C which needs unit conversion and dimensionless first (Liu et al. 2010). The Langmuir adsorption equilibrium constant, $K_{L,}$ can be considered to represent the affinity of a polymer for a particular surface. It can be related to the standard free energy of adsorption, ΔG^0_{ads}, from the flowing expression:

$$\Delta G^0_{ad} = -RT\,lnK_L \tag{2}$$

Where R is the general gas constant (8.314J/ (mol K) and T is the absolute temperature.

From the maximum adsorption density, the effective area occupied on the substrate surface per polymer chain, , can be calculated using Eq.3.

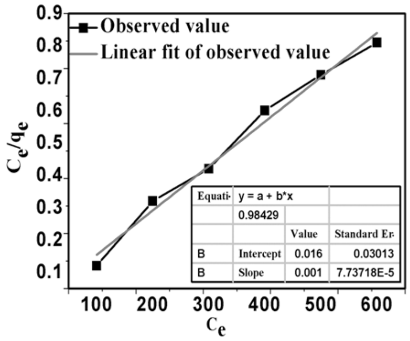
$$\sigma^0 = -\theta \frac{A}{n_2^s\, N_A} \tag{3}$$

N_A is the Avogadro number,is the fraction of the surface which is covered by CMC, A is the substrate surface area, and n_2^s is the number moles of CMC adsorbed per unit area of solid. The number of moles of CMC adsorbed per unit area of solid, n_2^s/A, is given by Eq.4.

$$\frac{\sigma_2^s}{A} = \frac{(x/m)_{max}}{M_W} \tag{4}$$

Where M_W is the molecular weight of the polymer (CMC). Therefore, the effective substrate area occupied per polymer molecule, σ°, can be calculated using Eq.5.

$$\sigma^0 = \theta \frac{M_W}{(x/m)_{max} N_A} \tag{5}$$



Equati-	y = a + b*x		
	0.98429		
		Value	Standard Er·
B	Intercept	0.016	0.03013
B	Slope	0.001	7.73718E-5

Fig. 3 Langmuir adsorption isotherm of CMC onto TiO_2-modified carbon at pH3, (30^0C)

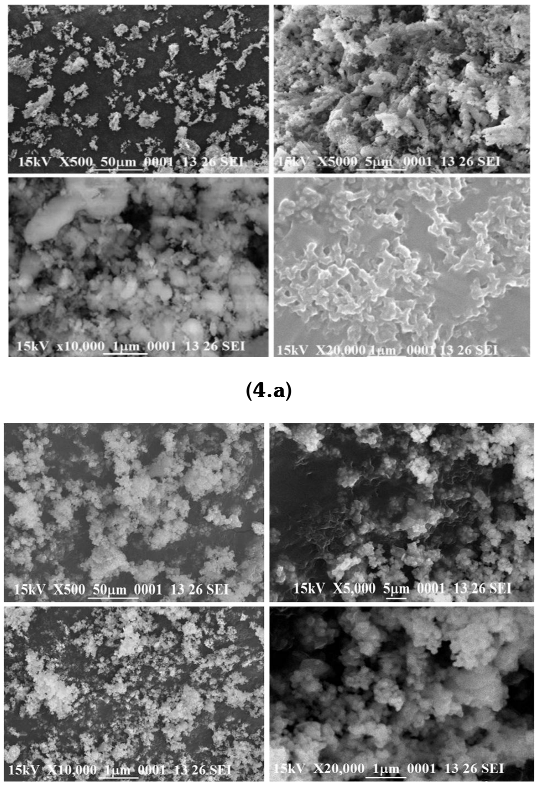
From Table S1, it is clear that ΔG^0_{ads}, evaluated for CMC, demonstrates that adsorption of CMC on TiO_2-modified carbon is highly favored, i.e. ΔG^0_{ads} negative. It is evident that the value of ΔG^0_{ads} is around −21 kJ/mol. As is well known, the free energy of hydrogen bond formation is about −25kJ/mol, which is very close to the ΔG^0_{ads} of the CMC in the present case. Additionally, if the hydrophobic interaction is the major force for adsorption, then a theoretical value around −50 kJ/mol might be expected for ΔG^0_{ads} (Miller et al. 1983), which is much greater than the calculated value. These results are also consistent with the literature (Wang and Somasundaran 2005) for adsorption of CMC at talc/water interface. These results further give added assurance for the major role of hydrogen bonding rather than hydrophobic force in binding mechanism of the CMC at carbon/water interface.

ELECTROKINETICS STUDIES

It is clear from the electrokinetic data shown in Fig. S4, that the surface of the TiO_2-modified carbon is negatively charged. Since PZC of adsorbent has been found 9.8, therefore at any pH below $pH_{ZPC,}$ the surface is positively charged and at pH above pH_{ZPC}, the surface is negatively charged. When the pH of the solution is lowered than pH_{ZPC}, the repeat units of polysaccharides are more easily attracted by the positively charged surface of TiO_2-modified carbon, favoring the accumulation of repeat units of CMC polymer on the surface and thus adsorption increases. On the other hand, when the pH of the solution is higher than pH_{ZPC} the repeat units of CMC are repelled by the negatively charged surface, hence adsorption decreases.

SEM ANALYSIS

The SEM images of PAMC (Singh and Mohan 2004) and TiO_2-modified carbon are shown in Figure 4, which clearly demonstrate the porosity and texture of TiO_2-modified carbon. It has been observed that modified adsorbent (TiO_2-modified carbon) retain the surface characteristics of its precursor (Blank PAMC or TiO_2) as shown in Fig. 4.a. However, with some remarkable modifications, the results (Fig. 4.b) obtained showed that there were displacement as the temperature of thermal decomposition of the modified adsorbent suggesting that the modification caused a difference in structure. The SEM micrographs (Fig. 4) show a spongy aspect, fibrous surface with irregular and heterogeneous structure with many pits and fissures through the surface prominent possibly due to powerful oxidizing agent H_2O_2, which caused some changes in the surface of the adsorbent.



(4.a)

(4.b)

Fig. 4 SEM Images at Different Magnifications: a. PAMC (blank), b. TiO_2-modified Carbon

ATTENUATED TOTAL REFLECTANCE FOURIER TRANSFORM INFRARED (ATR FTIR)

ATR *FTIR* spectroscopy clearly provides the evidence for specific functional groups on the surface of the TiO_2-modified carbon. Several characteristics bands were observed in the ATR FTIR spectrum (Fig. 5, 6). It is obvious that many existing groups in PAMC (Singh et al. 2016) (blank) are also present in the modified carbon, showing that modified material exhibits many of the same functional groups of PAMC (blank). It was observed that the infrared spectra of TiO_2-modified carbon which overlapping with PAMC (source material) so that there are new peaks as observed in 3832.20-3425.4, 1632.21, 1570, 1046.50, 600.23, 500.30 cm^{-1}.

The broad and strong bands at 3832.20-3425.4 cm^{-1} have been assigned because of bonded hydroxyl (-OH) or amine ($-NH_2$) groups. The band 1632.21 can be ascribed to –C=O stretching. The band around 1570 cm^{-1} can be ascribed to –C=C. The band at 1046.50 cm^{-1} is due to C-O of carbonyl groups. The stretching bond corresponding to Ti-O-Ti is clearly in the region of 509 cm^{-1} (Yu and Yunhua 2013). The band around 620.23cm^{-1} is attributed to the Ti-O-C vibration which indicates that TiO_2 (Dugasa P25) were chemically bonded with carbonized carbon in TiO_2-modified carbon.

The ATR FTIR spectrum of CMC shown in Fig.S5 illustrate a band at 2920.8 cm^{-1} which is attributed to C–H stretching of the $–CH_2$ groups. The band at 1610.32 cm^{-1} is attributed to ring stretching of glucose. Additionally, there are bands in 1350–1450 cm^{-1} due to symmetrical deformations of CH_2 and COH groups. The appearance of peaks at 1060 and 1010 cm^{-1} is due to primary alcoholic $–CH_2OH$ and CH_2 twisting vibrations, respectively. The ring stretching and deformation of α-D-(1–4) and α-D-(1–6) linkages appears at around 714-610.70 cm^{-1}.

The ATR FTIR spectrum of CMC adsorbed onto carbon/ water interface shown in Fig. 5 clearly shows the characteristics band at 1632.23 cm−1 due to $–COO^-$ of the carboxyl groups of CMC .appeared to be less sharp and shifted to 1650 cm−1 after adsorption. Additionally, Fig. 6 clearly illustrates Ti–O–Ti band at 1046.50 cm^{-1} which splits into sharp peaks at around 1000–500 cm^{-1} after CMC adsorption onto modified carbon/ water interface. The difference in ATR FTIR spectrum is attributed to the hydrogen bond formation between carboxylate (COO^-) ions of the CMC and surface hydroxyls of TiO_2 modified carbon. Since, adsorption experiments were conducted at pH 3.0, under such condition the CMC gets ionized (pKa = 3.3, Crowdhury and Neale, 1963) and provides COO^- ions. It is important to mention here that primary alcoholic $–CH_2OH$ of the CMC are not available for hydrogen bonding with surface because these groups are already involved in extensive intramolecular hydrogen bonding within the structure.

The appearance of XPS peak at **286.7 eV** (Fig.12) attributes the presence of hydroxyls as evidenced by high resolution XPS of TiO_2 modified carbon surface. Therefore, the possibility of hydrogen bonding between carboxylate ions and –OH surface hydroxyls cannot be ruled out. This observation was further confirmed by the fact that in the presence of urea amount of adsorption reduced significantly. The changes in the infrared bands in the region 1000 –500 cm−^{1}, attributed with the C–O stretch coupled to the C–C stretch and O–H deformation, were significant and therefore support strong hydrogen bonding of CMC to the carbon/water interface.

ELECTROKINETICS STUDIES

It is clear from the electrokinetic data shown in Figure 8, that the surface of the MPP is negatively charged. Since ZPC of the modified adsorbent (MPP) has been found 8.2, therefore at any pH below $pH_{ZPC,}$ the surface is positively charged and at pH above pH_{ZPC}, the surface is negatively charged. When the pH of the solution is lowered than pH_{ZPC}, the repeat units of CMC are more easily attracted by the positively charged surface of MPP, favouring the accumulation of repeat units of CMC on the surface and thus adsorption increases. On the other hand, when the pH of the solution is higher than pH_{ZPC} the repeat units of CMC are repelled by the negatively charged surface, hence adsorption decreases.

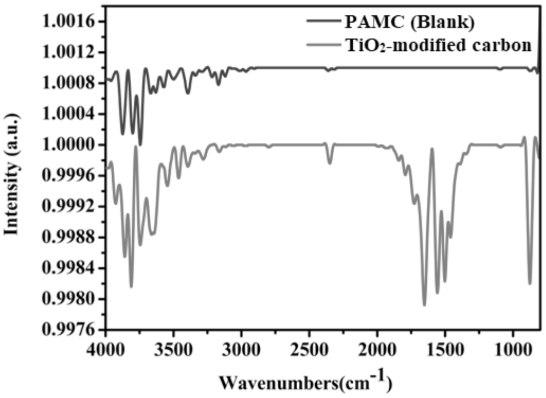


Fig. 5 ATR FTIR spectra of PAMC and TiO_2-modified carbon

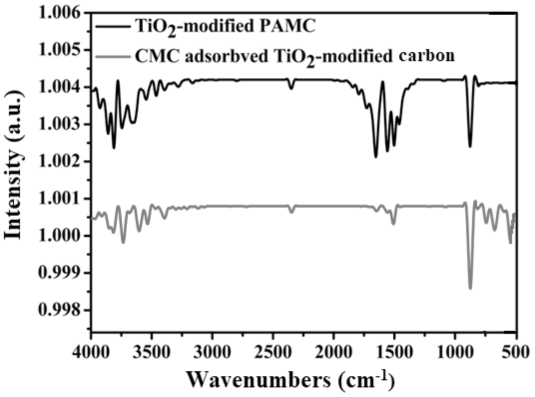


Fig. 6 ATR FTIR spectra of TiO_2-modified carbon and CMC adsorbed TiO_2-modified carbon

X-RAY DIFFRACTION

pXRD spectrum shown in Fig.S6 illustrates that the treated carbon from de-oiled mustered cake and modified with TiO_2 under optimum preparation condition is crystalline in structure**.** There are seven broad peaks centered on 2θ value of 25^0, 30^0, 37^0, 47^0, 52^0, 54^0 and 63^0. 2θ $=68^0$ is not clearly described.

BET SURFACE AREA

The Brunauer–Emmett–Teller (BET) surface area was measured by means of standard BET (Brunauer et al. 1938) equation. The pore size distribution was calculated employing Barrett-Joyner –Halenda (BJH) model (Barrett et al. 1951) for N_2 adsorption isotherm. The BET analysis reveals that TiO_2-modified carbon had a surface area ($\boldsymbol{S}_{BET}$) = 18.845 $m^2\ g^{-1}$, which was primarily contributed by mesopores. The average pore diameter and total pore volume of TiO_2-modified carbon were found to be 10.564 nm and $0.0497 cm^3 g^{-1}$, respectively, which is an indicative of its mesopores character as defined by Dabrowski (2001), is as follows: micropores, <2nm; mesopores, 2-50nm; macrospores, >50nm. (Fig. S7).

FLUORESCENCE SPECTROSCOPY

Fluorescence study (Fig. S8) clearly illustrate no evidence for hydrophobic domain formation upon the adsorption of CMC at TiO_2-modified carbon aqueous interface suggesting instead the governing role of hydrophilic forces. On increasing the concentration of CMC the polarity parameter decreases, suggests that no hydrophobic domain at the TiO_2-modified carbon –aqueous interface; instead, the fluorescence results suggest the formation of hydrophilic domains for the adsorption of CMC on TiO_2-modified carbon.

AFM ANALYSIS

From AFM imaging (McIntire et al. 1995; Gunning et al. 1996; Wilkinson et al. 1999; Rath and Subramanian 1997; Chen 2015) of CMC, it is clear that CMC is more adsorbed on mica surface at pH 3.0 than that pH 9.0 at the same concentration (200ppm). Fig. 8, 9 indicates that electrostatics interactions do affect the adsorption of CMC on a solid surface. Further, the average thickness of adsorbed cluster is around 1 nm, it shows that a flat conformation of this polymer on the solid surface. On the other hand, AFM imaging of PAMC (blank) and TiO_2-modified carbon demonstrate that the roughness of the surface increases which favors adsorption of CMC. The average roughness of PAMC was 92nm while the roughness of TiO_2-modified carbon was 248 nm.

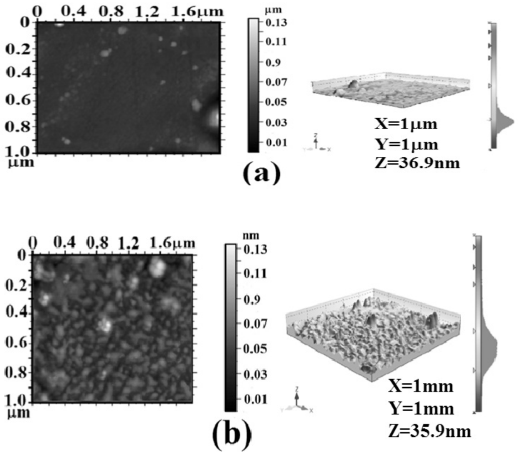


Fig. 7 AFM images of (a) PAMC; Average roughness: 92 nm (b) TiO_2-modified carbon: Average roughness: 248nm

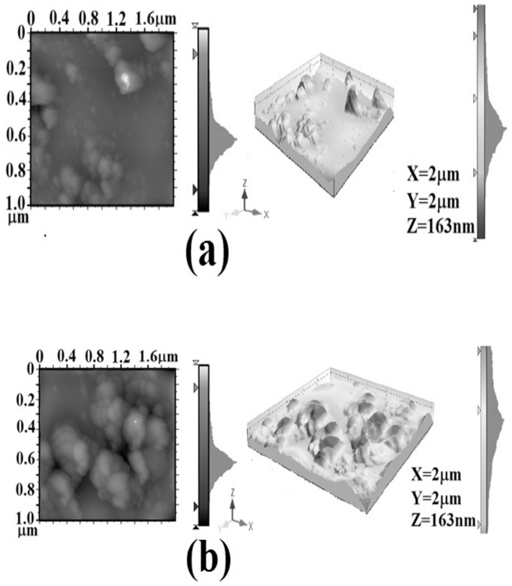


Fig. 8 AFM Images of CMC Adsorbed on Mica at (a) pH 9.0, (b) pH 3.0,

X-RAY PHOTOELECTRON SPECTROSCOPY MEASUREMENTS

To determine the chemical composition of the PAMC, TiO2 - modified carbon and TiO2 -modified carbon adsorbed CMC XPS analysis was performed. The surveys scan of PAMC in (Fig. 9) demonstrates that its oxygen content is around 17.4 %, suggesting the containing of abundant surface oxygenic functional groups. In the C 1s XPS spectra of PAMC (Fig. 10.), the peaks at 284.8, 286.7, and 288.9 eV are ascribed to the sp2 hybridized (C–C), alcoholic (C–OH) and carbonyl (C=O) carbon atoms, respectively.

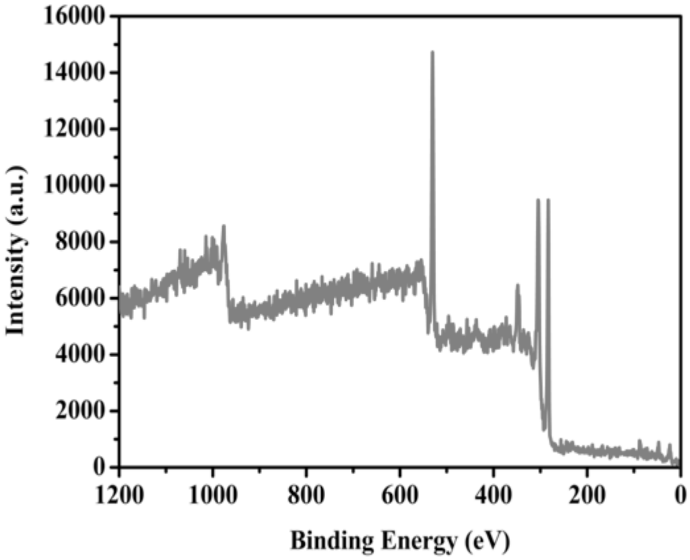


Fig. 9 XPS survey AlKα PES of PAMC,

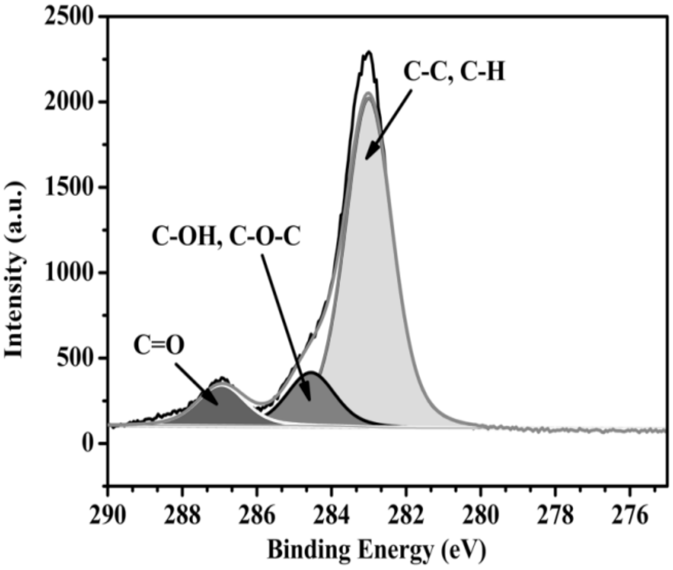


Fig. 10 High-resolution C1s XPS spectra PAMC

The XPS survey scans of TiO_2 - modified carbon (Fig. 11.) show the typical spectra of TiO_2 (P25), and the more intense feature peak of C1s in TiO_2 - modified carbon is attributed to the carbon layer of the hybrid. With regard to the C1s XPS spectra of TiO_2 - modified carbon (12), aside from the above listed characteristic peaks, it is evidently noticed that an additional peak emerges at the binding energy of 283.5 eV, which is higher than that of titanium carbides (Ti^{4+}–C) and should be assigned to the carbon bonded with oxygen-deficient titanium ion (Ti^{3+}–C) revealing the distinctive chemically bonded carbon/ TiO_2-modified carbon.

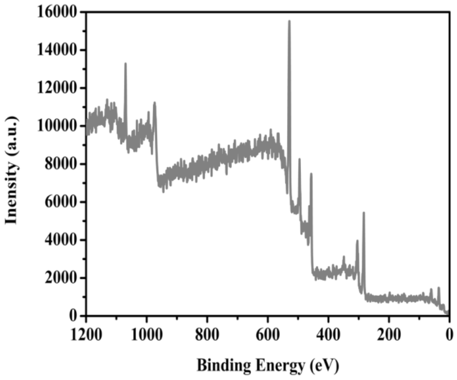


Fig. 11 XPS survey AlKα PES of TiO$_2$-modified carbon

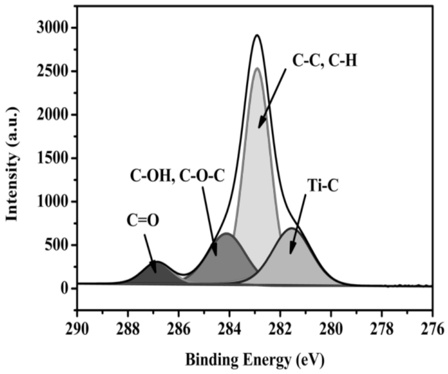


Fig. 12 High-resolution C1s XPS spectra of TiO$_2$-modified carbon

In addition, the atomic ratios of O: C for PAMC and TiO$_2$ - modified carbon are 0.21 and 0.17, respectively, suggesting the decreased oxygen content of coated PAMC on TiO$_2$ – modified carbon. To clarify the chemical state of titanium ions, the Ti 2p spectra of TiO$_2$ - modified carbon was taken Fig. 13.

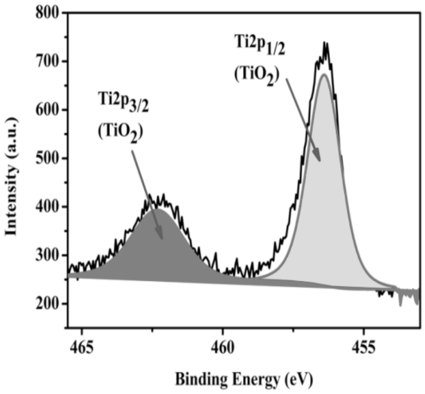


Fig. 13 High-resolution XPS spectra of Ti 2p of C (Is) C1s XPS spectra TiO$_2$-modified carbon

The typical Ti^{4+} 2p$^{3/2}$ and 2p$^{1/2}$ peaks of T-O located at 458.8 and 464.6 eV shifted negatively to 458.6 and 464.4 eV for TiO$_2$ - modified carbon, respectively, and two weak shoulder peaks at 457.1 and 462.3 eV revealed, corresponding to the presence of the reduced titanium (Ti^{3+}).Based on these characterizations, the possible formation partially bonded TiO$_2$/ TiO$_2$ - modified carbon is confirmed. The XPS survey scan of CMC was also performed as shown in Fig. 14, as well as high-resolution C 1s XPS spectra of CMC (Fig. 15), was taken.

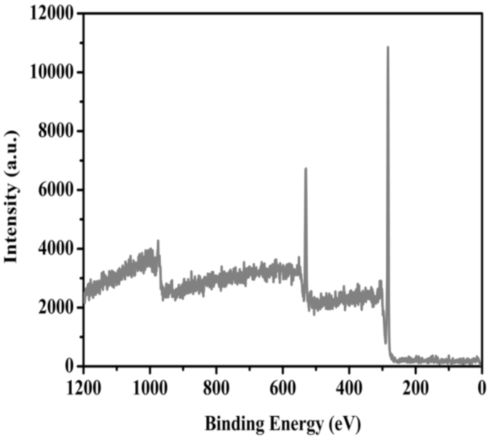


Fig. 14 XPS survey AlKa PES of CMC

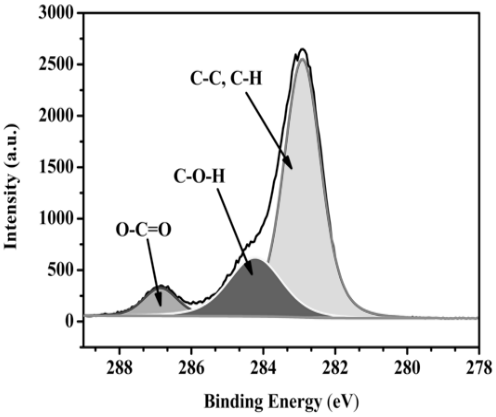


Fig. 15 High-resolution C1s XPS spectra carboxymethyl cellulose

The CIs XPS spectrum of CMC is deconvoluted into 3 peaks C-C, CC-H (283.60), O-C (284.34 and O-C=O (287.01).The approach involves the subtraction of a Shirley background followed by a charge correction referenced to C1s of adventitious carbon at 285.0 eV.

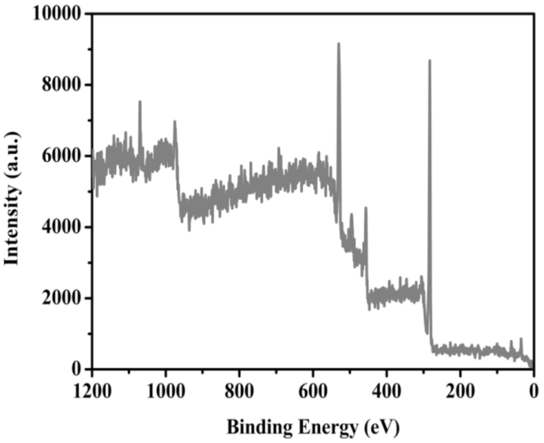


Fig. 16 XPS survey AlKa PES of TiO$_2$-modified carbon and adsorbed CMC

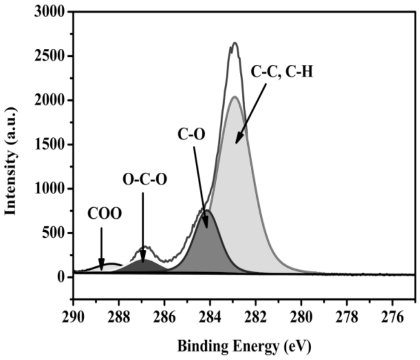


Fig. 17 High-resolution XPS spectra of C1s after adsorption of CMC showing an increase in carbon-oxygen functional groups (C-O and C = O).

After the adsorption of CMC onto the surface of TiO_2 - modified carbon both XPS survey scan (Fig. 16.) and high-resolution C Is XPS spectra (Fig. 17) was taken in which binding energy is different because the chemical shifts are related to electron density changes. This is due to available hydroxyl groups on TiO_2 - modified carbon interacts with carboxylate ion of CMC resulting an increase in carbon-oxygen functional groups (C-O and C = O) of TiO_2- modified carbon.

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CONCLUSIONS

The present study leads to following important conclusions:

i. The particle size study confirms that TiO_2-modified carbon falls on the mesoporous domain. The typical specific surface area of TiO_2-modified carbon was found as S_{BET} = 18.845 m^2g^{-1}.

ii. It was found that the adsorption of CMC on TiO_2-modified carbon affected by changes in pH and ionic strength. These observed results conclude that the electrostatic force plays an important role in the binding of CMC at TiO_2-modified carbon /water interfaces.

iii. The results obtained from the ATR FTIR analysis provided useful information on spectral changes which are assigned with hydrogen bonding between CMC and TiO_2-modified carbon The changes in the infrared bands in the region of 1000–1080 cm^{-1}, associated with the C–O stretch coupled to the C–C stretch and O–H deformation, were significant and thus support strong hydrogen bonding of CMC on carbon/water interface.

iv. Fluorescence spectroscopy supports that there is no existence of hydrophobic domain upon the adsorption of CMC at carbon/water interfaces, suggesting instead the governing role of hydrophilic forces.

v. Urea, a hydrogen bond breaker, reduced the amount of adsorption of CMC on TiO_2-modified carbon significantly. This result also supports a mechanism involving hydrogen bonding rather than a hydrophobic one.

vi. Langmuir adsorption isotherm studies further support the hydrogen bonding as the dominant force for CMC adsorption since the adsorption free energy of CMC is close to that of hydrogen bond formation.

vii. AFM analysis confirms that CMC was adsorbed in a very flat conformation on the TiO_2-modified carbon surface per polymer chain.

viii. XPS analysis confirms that the binding of titanium with carbon of mustard cake and is not available for binding with CMC at pH 3.0. The survey scan and high resolution of C1S XPS spectra confirm that OH groups available onto TiO_2-modified carbon surface interacts with carboxylate ion of the CMC.

Thus, the present study provides substantial evidences to prove beyond doubt that adsorption of CMC on carbon/water interface depends on experimental conditions and governs by a complex interplay of electrostatic interaction, hydrogen bonding and hydrophobic force.

ACKNOWLEDGMENT

The authors are thankful to IIT Kanpur for XPS, AFM and XRD facilities and SIL, DAC, BBAU for BET surface characterization facility. The financial support to (A.K.) from UGC (173/Conf./DAC/BBAU,13/10/16) is gratefully acknowledged.

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Supplementary Material

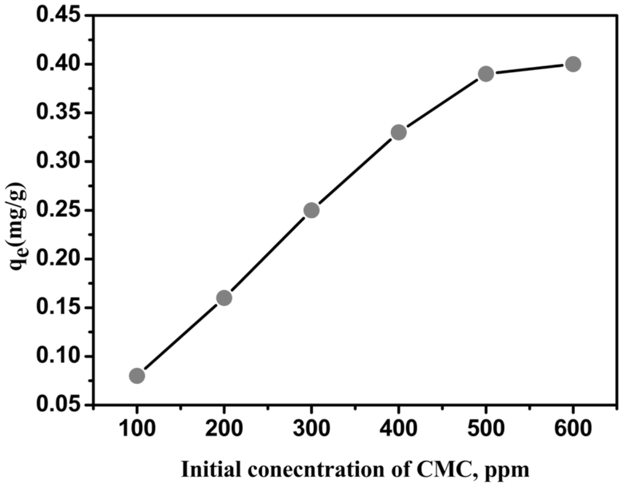


Fig. S1 Effect of concentration on adsorption isotherm of CMC on TiO_2-modified carbon

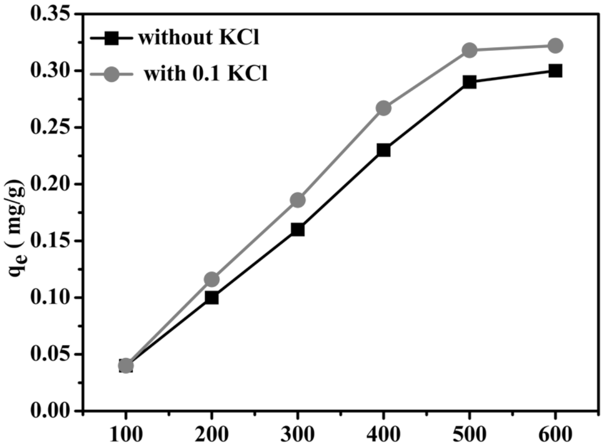


Fig. S2 Effect of ionic strength on adsorption isotherm of CMC on TiO_2-modified carbon

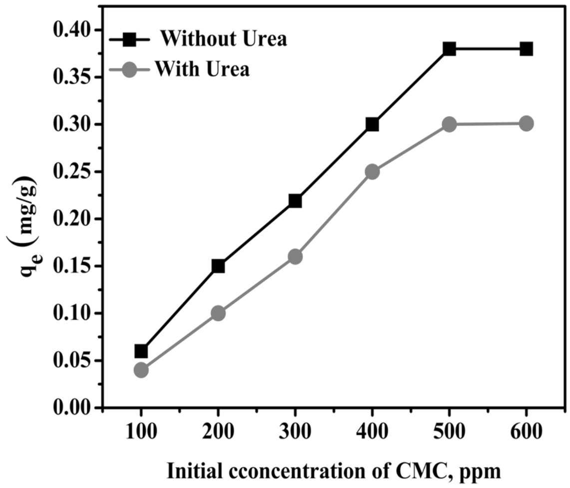


Fig. S3 Effect of urea on adsorption isotherm of CMC on TiO_2-modified carbon

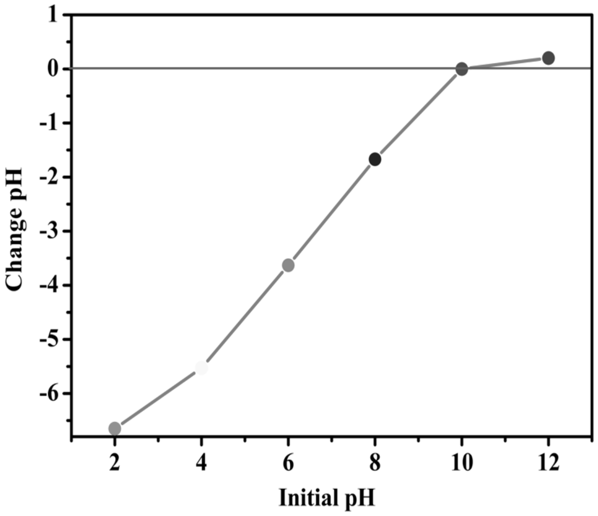


Fig. S4 Point of zero charge of TiO_2-modified carbon addition method

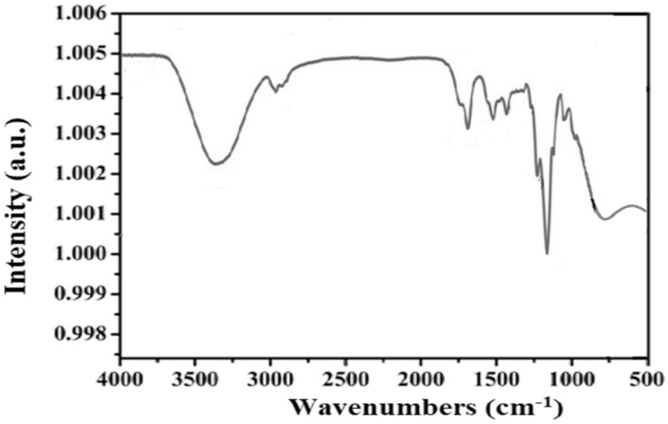


Fig. S5 ATR FTIR spectrum of carboxymethyl cellulose

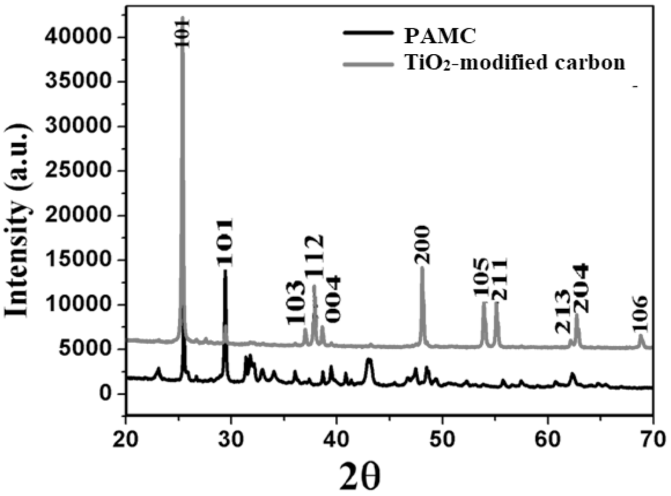
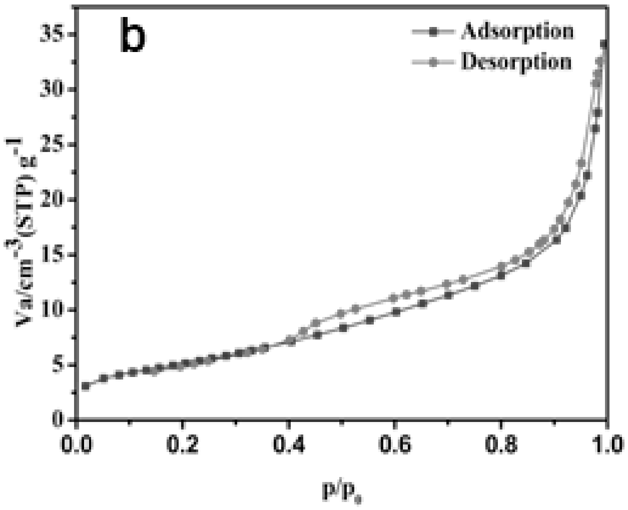


Fig. S6 pXRD spectra of PAMC and TiO_2-modified carbon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Desorption
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15
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30
35
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0.2
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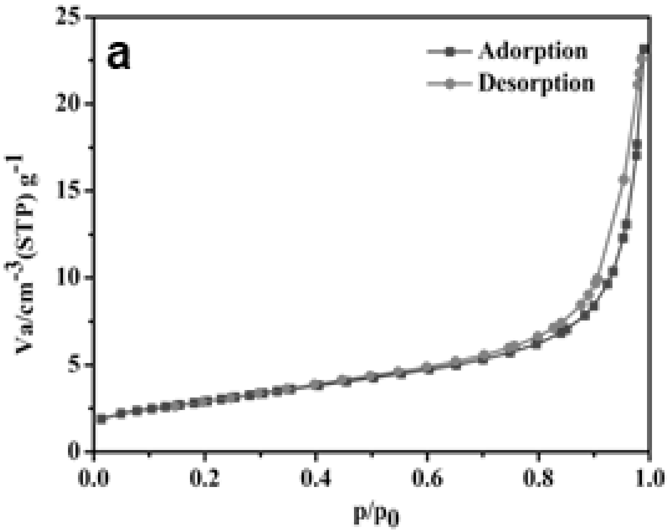
p/p$_0$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Adorption
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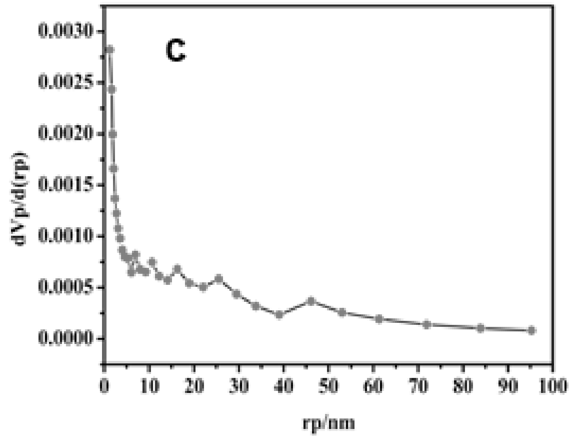
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dVp/d(rp)
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rp/nm

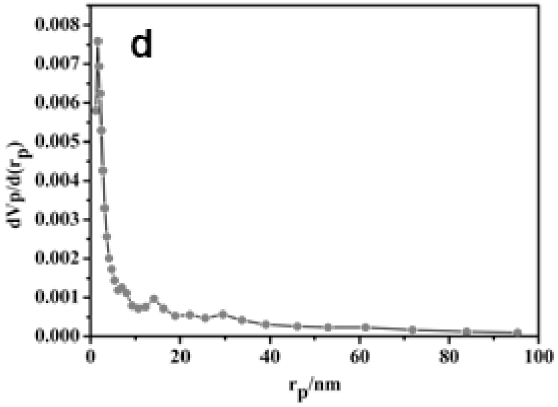

Fig. S7 The nitrogen adsorption/desorption isotherms of (a).PAMC and (b). TiO2-modified carbon and the corresponding pore size distribution of (c).PAMC and (d). TiO2-modified carbon

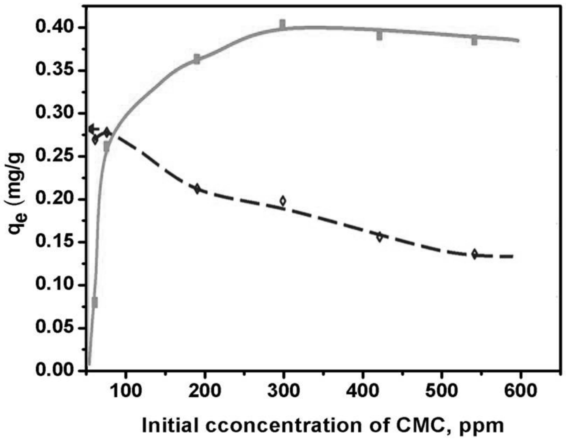

Fig. S8 Fluorescence spectra for CMC and TiO_2-modified carbon interface

FRP-02

A Thermodynamic and Comparative Study of Pharmacetical Drug (Paracetamol) by Ir(III) and Pd(II) Catalysed Oxidation in Acidic Medium($HClO_4$): Kinetic Model

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Abstract—A comparative study of Pharmacetical drug (Paracetamol) by Ir(III) and Pd(II) catalysed oxidation in acidic medium ($HClO_4$] at 35 ^{0}C to 45 ^{0}C. The reaction is carried out in the presence of mercuric acetate as a scavenger for bromide ion. 1-carboxy cyclohexane l-acetic acid was obtained as the oxidation product and identified chromatographically. The rate law followed a first order and zero order dependence with respect to $KBrO_3$ and potassium chloride [KCl] respectively. The reaction followed first order with respect to Ir(III) and Pd(II) chloride. Negligible effect of $[Hg(OAc)_2]$ and ionic strength of the medium was observed. The rate of reaction decreased with increasing $[H^+]$ was observed for the oxidation of paracetamol. Rate of reaction exhibits fractional positive order kinetics with respect to [PA]. The values of rate constants observed at different temperatures (30 to 45^{0}C) were utilized to calculate the activation parameters. Quinoneoxime and acetic acid have been identified as main oxidation products of the reactions. Feasible mechanism is proposed which are be composed with the kinetics, stochiometry and product of the reaction. The rate law has been derived from obtained kinetic data.

Keywords: Kinetics, Ir(III) Chloride, Pd(II) Chloride Oxidation, Paracetamol, Potassium Bromate, Acidic Medium.

INTRODUCTION

The transition metal catalysed reactions are important for the chemical industry from both practical and economic point of view. Transition metal ions are found to be good catalysts and their complexes are also able to catalyze a wide variety of reactions like hydrogenation, oxidation and polymerization. The applications of transition metal catalyst such as Ru(III)[1-2], Rh(III)[3-4], Cu(II)[5-6], and Pd(II)[7-8] in kinetic studies of redox reaction involving organic substrate are reported in literature. It was found that these catalysts work efficiently in both acidic and alkaline media. The use of Ir(III) chloride as a non-toxic and homogenious catalyst has been reported[9-11]. The reaction path depends not only upon the nature of the oxidant and the nature of the substrates but also upon the ways in which reactive species of transition metal ion forms complex with the reactant molecules before changing into final products under experimental conditions.Oxidant such as NBS[13-14], NBA[14-15], Periodate[16-17], and iodate[18-19], have been successfully utilized in kinetic and mechanistic investigations of various organic substrate. Amongst various inorganic oxidants, iodate has been used as an oxidant in the uncatalyzed oxidation of oxalic acid[20], acetophenone[21], benzeldehyde[22]. Singh et al [23-26] have introduced various reports in the literature regarding the oxidation of reducing sugars involving Ir(III) as homogenious catalyst. Potassium bromate is known to be a powerfull oxidizing agent with redox potential 1.44 volts and has been used widely in the oxidation of several organic substrates [27]. Potassium bromate is used for oxidation of uncatalyzed reactions by several workers.[28-29] Uncatalyzed reactions of aldoses and aldosamines[30], carbohydrates[31] compound oxidation by potassium bromate has also been reported. Ir(III) catalyzed cyclic alcohols[32], cyclic ketones[33] oxidation by potassium bromate has also been reported. Comparatively Ir(III) catalyzed oxidation has been dealt than other catalyst and scant attention has been paid with potassium bromate as an oxidant. The kinetics of paracetamol (PAM) oxidation has been studied both spectrophotometrically and iodometrically. Spectrophotometric determination of paracetamol in drug formulation has been a subject of several investigators. [34-42].. It is antipyretic and analgesic compound of high therapeutic value.[43-44] It is also used as an intermediate for pharmeceutical (as a precursor in penicillin) and azo dye.[45-47] Oxidation reactions are important in the synthesis of organic compounds, create new functional groups or modify existing functional groups in a molecule.[48-49] Various advanced oxidation processes such as electrochemical[50-52] ozonation and H2O2 / UV oxidation[53-56] have been employed to remove aqueous paracetamol. Several authors have performed studies using Pd(II) because of the commercial importance of reactions catalyzed by Pd(II). The kinetics for the oxidation of ethylene by aqueous Pd (II) is an example [57-58]. In this study the effect of chloride ion on the reaction rate was studied in order to establish the active species of the catalyst. Generally the mechanism of catalysis depends on the nature of the substrate, the oxidant, and other experimental conditions [59-60]. In most of the catalytic studies for organic transformations, the nature of active form of Pd(II) remain obscure. The kinetic methods of analysis are highly sensitive, selective, simple, accurate, and less expensive. The present study examines, in detail the kinetic and mechanistic aspects of the Ir(III) catalyzed oxidation of paracetamol by $KBrO_3$ in acidic media with the following objective. In this paper it has been tried to consolidate the various work done on the well-known drug that finds extensive application in pharmaceutical industries in the last few decades. In most of the catalytic studies for organic transformations, the nature of active form of Pd(II) remain obscure. The kinetic methods of analysis are highly sensitive, selective, simple, accurate, and less expensive. In recent years, several kinetic Paracetamol (4-hydroxyacetanilide or acetmidophenol) is a well known drug that is having extensive appliction in pharmaceutical industries. The present study examines, in detail the kinetic and mechanistic aspects of the Ir(III) / Pd(II) catalyzed oxidation of paracetamol by $KBrO_3$ in acidic media with the following objective.

i. To ascertain the reactive species of the catalyst and the oxidant.

ii. To deduce the rate law consistent with the kinetic results.

iii. Identify the oxidation products.

iv. To estimate activation parameters.

v. To elucidate the plausible reaction mechanism based on the observed reacion rate law and stoichiometry

MATERIAL AND PROCEDURE

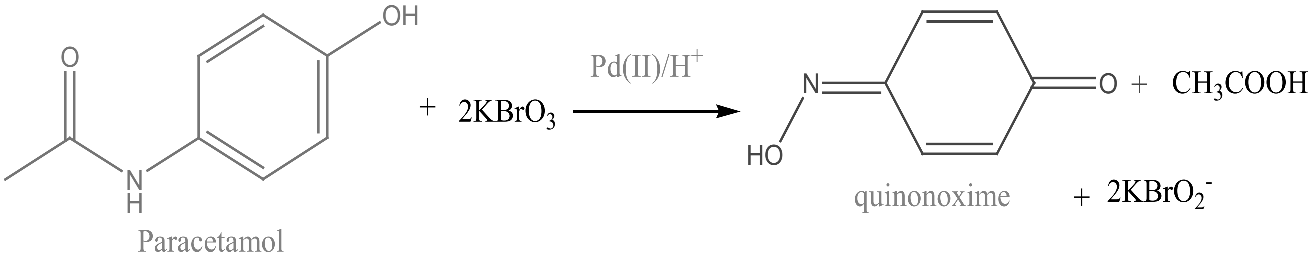
Materials

Aqueous solution of Paracetamol (CDH), potassium bromate (S.D. Fine A.R.) and mercuric acetate (E. Merck) were prepared by dissolving the weighed amount of sample in triple distilled water. Perchloric acid (60% E. Merck) was used as a source of hydrogen ions. Iridium (III) chloride and palladium chloride (Johnson Matthey) was prepared by dissolving the sample in hydrochloric acid of known strength. All other reagents of analytical grade were available. Sodium perchlorate (E. Merck) was used to maintain the ionic strength of the medium. The reaction stills were blackened from outside to prevent photochemical effect.

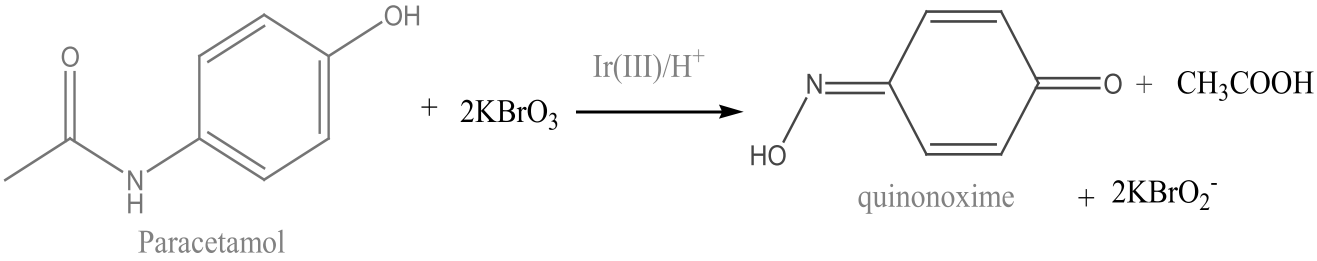
Kinetic Procedure

A thermostated water bath was used to maintain the desired temperature within ± 0.1 °C. Calculated amount of the reactants i.e. paracetamol, perchloric acid, mercuric acetate, Ir (III)/Pd(II) chloride, KCl and water, except potassium bromate were taken in a reaction vessel which was kept in a thermostatic water bath. After allowing sufficient time to attain the temperature of the experiment, requisite amount of potassium bromate solution, also thermostated at the same temperature was rapidly pipetted out and run into the reaction vessel. The total volume of reaction mixture was 50 mL in each case. Aliquots (5mL) of the reaction mixture were pipetted out at regular intervals of time and poured in to a conical flask containing 5 mL of 4 % KI solution and 5 mL of dilute sulfuric acid. The liberated bromine equivalent to consumed oxidant was estimated with standard sodium thiosulphate solution using starch as an indicator. The rate of reaction (-dc/dt) was determined from the slope of the tangent drawn at a fixed [BrO_3^-] in each kinetic run. The order of reaction in each reactant was measured with the help of log plot of (-dc/dt) versus concentration of the reactants.

Determination of stoichiometry and product analysis of Pd(II) chloride for the oxidation of paracetamol.



Determination of stoichiometry and product analysis of Ir(III) chloride for the oxidation of paracetamol



Different sets of the reaction mixture containing Paracetamol, Ir(III)/Pd(II) chloride, and $HClO_4$ with excess $KBrO_3$ were equilibrated for 72 h at 303 K. Estimation of unconsumed $KBrO_3$ in each set revealed that for the oxidation of 1 mol of Paracetamol, 2 mols of $KBrO_3$ were consumed. Accordingly, the stoichiometry equation may be expressed as the reaction products were extracted with ether after completion of the reaction (monitored by TLC). Evaporation of the ether layer was followed by column chromatography on silica gel using a gradient elution (from dichloromethane to chloroform). After the initial separation, the products were further purified by recrystallization. Acetic acid and quinine oxime were identified as oxidation products of Paracetamol and $2KBrO_2$ was the reduction product of $KBrO_3$. The quinone oxime was identified by its IR spectrum (1652 cm-1, C=O stretching; 1615 cm-1, C=N stretching of oxime; 3332 cm^{-1}, O-H stretching). Identification was further confirmed by its melting point of 131^{0}C (literature mp 132^{0}C)

RESULT AND DISCUSSION

The kinetic results were collected at several initial concentrations of reactants (Table). The initial rate (-dc/dt) in each kinetic run was calculated by the slope of tangent drawn at fixed time for the variation of [$KBrO_3$] while in the variation of other [reactants], tangents drawn at fixed [$KBrO_3$] which was written as [$KBrO_3^*$]. The first order rate constant K_1 was calculated as

$$\frac{K_1 = -\,(dc/dt)}{[KBrO_3^*]}$$

Each kinetic run was studied for two half lives of the reaction. The observed rates of reaction were reproducible with in ± 5% in replicate kinetic run. The order of reaction in each reactant was determined with the help of log-log plot of (-dc/dt) vs. Concentration of reactant. First order rate constant k_1 i.e. (-dc/dt/$KBrO_3$*) were calculated from the plots of unconsumed potassium bromate vs. time. The comparative plots of log(-dc/dt) versus log (oxidant) were linear indicating first order dependence on $KBrO_3$ (Fig-1). Insignificant effect on the rate was observed on increasing the concentration of [Cl^-] indicating zero order in [KCl], i.e. potassium chloride (Table-2). The rate of reaction increases as the concentration of Iridium (III) chloride and Pd(II) chloride is increased, It was observed that values of (-dc/dt) were doubled when the concentration of iridium(III)/Pd(II) was made two times, showing first order dependence on $IrCl_3$ / $PdCl_2$ indicating first order of catalyst i.e. Ir(III) chloride and Pd(II) chloride (table-1) and comparative graph (fig-3). Kinetic result obtained on varying concentrations of substrate indicates fractional positive order of paracetamol, which implies that rate of reaction increases when the concentration of [PA] is increased with both catalyst (table-1) and (fig-2) .With increasing the concentration of [H^+], the value of reaction rate decreases for both catalyst (Table-2) and (fig-4). This shows negative effect of the reaction rate with respect to [H^+] on the rate of oxidation of paracetamol. The rate measurements were taken at 30^0-45^0C and specific rate constants were used to draw a comparative graph plot of log k vs. 1/T which was linear (Fig-5).

Table 1: Effect of variation of oxidant, substrate, catalyst at 35^0C

[Oxidant] x 10^3M (Potassium bromate	[Substrate]x 10^2M (Paracetamol)	[Pd(II) / Ir(III)] x 10^5M	(-dc/dt)x10^7ML^{-1}s^{-1} Pd(II)	Ir(III)
0.80	1.00	11.2	1.92	4.30
1.00	1.00	11.2	2.60	5.20
1.25	1.00	11.2	2.82	6.45
1.69	1.00	11.2	3.81	8.65
2.50	1.00	11.2	5.32	12.80
5.00	1.00	11.2	10.60	25.50
1.00	0.40	11.2	1.32	3.80
1.00	0.50	11.2	1.60	4.30
1.00	0.66	11.2	2.10	4.62
1.00	1.00	11.2	2.60	5.20
1.00	2.00	11.2	4.25	6.65
1.00	4.00	11.2	6.20	8.25
1.00	1.00	5.60	1.33	2.56
1.00	1.00	11.2	2.60	5.20
1.00	1.00	16.8	4.60	10.30
1.00	1.00	22.4	5.18	15.32
1.00	1.00	33.6	8.35	20.40
1.00	1.00	44.8	10.21	25.90

Solution Condition: [$HClO_4$] = 1.00 X 10^{-3} M, [KCl] = 1.00 X 10^{-3} M, [$Hg(OAC)_2$] = 1.25 X 10^{-3} M

Table 2: Effect of variation of perchloric acid ($HClO_4$), potassium chloride(KCl), mercuric acetate [$Hg(Ac)_2$] and sodium per chlorate at 35^{0}C

[$HClO_4$] x10^3M	[KCl] x 10^3M	[$Hg(OAc)_2$] x 10^3M	$NaClO_4$ x 10^3M	(-dc/dt) x $10^7ML^{-1}s^{-1}$	
				Pd(II)	Ir(III)
0.83	1.00	1.00	1.00	3.12	5.60
1.00	1.00	1.00	1.00	2.60	5.20
1.25	1.00	1.00	1.00	2.41	4.60
1.67	1.00	1.00	1.00	2.00	4.25
2.50	1.00	1.00	1.00	1.22	3.60
5.00	1.00	1.00	1.00	0.82	2.95
1.00	0.83	1.00	1.00	2.23	4.90
1.00	1.00	1.00	1.00	2.60	5.20
1.00	1.25	1.00	1.00	2.00	4.52
1.00	1.67	1.00	1.00	2.81	5.45
1.00	2.50	1.00	1.00	2.52	5.12
1.00	5.00	1.00	1.00	2.42	4.72
1.00	1.00	0.83	1.00	2.21	4.52
1.00	1.00	1.00	1.00	2.60	4.93
1.00	1.00	1.25	1.00	2.60	5.20
1.00	1.00	1.67	1.00	3.00	4.62
1.00	1.00	2.50	1.00	2.42	5.55
1.00	1.00	5.00	1.00	2.51	5.32
1.00	1.00	1.00	0.83	2.00	5.00
1.00	1.00	1.00	1.00	2.60	4.63
1.00	1.00	1.00	1.25	2.00	5.20
1.00	1.00	1.00	1.67	2.22	5.10
1.00	1.00	1.00	2.50	2.10	5.63
1.00	1.00	1.00	5.00	2.00	5.11

Solution Condition: [Oxidant ($KBrO_3$)] = 1.00 X 10^{-3} M, [Paracetamol(PA)] = 1.00 X 10^{-2} M, [Ir (III)and Pd(II) Chloride] = 11.2 X 10^{-5} M

Role of Entropy of Activation and other Activation Parameters

The value of energy of Activation (ΔEa) Arrhenius factor (A), entropy of activation (ΔS*) and free energy of activation (ΔG*) were calculated from rate measurement at 30^0, 35^0, 40^0, 45^0C and these values have been recorded in Table-3. Moderate ΔH* and ΔS* values are favourable for electron transfer reaction. The value of ΔH* was due to energy of solution changes in the transition state. The high positive values of change in free energy of activation (ΔG*) indicates highly solvated transition state, while fairly high negative values of change in entropy of activation(ΔS*) suggest the formation of an activated complex with reduction in the degree of freedom of molecule. The observed modest enthalpy of activation and a higher rate constant for the slow step indicates that the oxidation presumably occurs via an inner-sphere mechanism. This conclusion is supported by earlier observations. The high positive values of change in free energy of activation (ΔG*) indicates highly solvated transition state, while fairly high negative values of change in entropy of activation(ΔS*) suggest the formation of an activated complex with reduction in the degree of freedom of molecule [61]. The activation parameters evaluated for the catalyzed and uncatalyzed reaction explain the catalytic effect on the reaction. Entropy of activation plays an important role in the case of reaction between ions or between an ion and a neutral molecule or a neutral molecule forming ions. When reaction takes place between two ions of opposite charges, their union will results in a lowering of net charge, and due to this some frozen solvent molecules will released with increase of entropy but on the other hand when reaction takes place between two similarly charged species, the transition state will be more highly charged ion and due to this, more solvent molecules will be required for seprate the ions, leading to decrease the entropy.

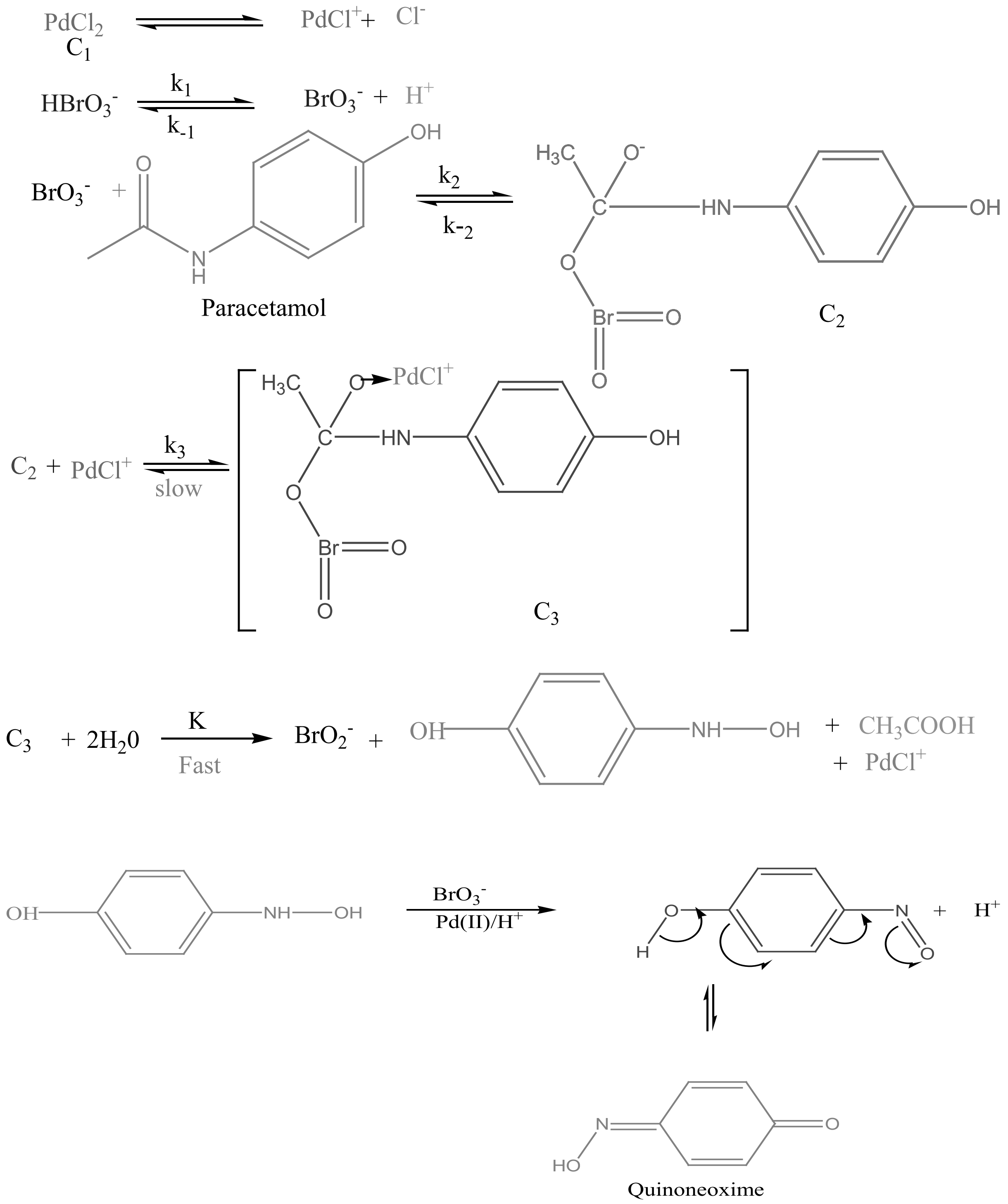
Table 3: Activation Parameters for Pd(II) / Ir(III) Chloride Catalyzed Oxidation of Paracetamol by $KBrO_3$ at 35^0C

Parameter	Temperature(T^0C)	Paracetamol(-dc/dt)x 10^7	
		Pd(II)	Ir(III)
$k_1 \times 10^4 s^{-1}$	30^0	1.55	3.70
$k_1 \times 10^4 s^{-1}$	35^0	2.60	5.20
$k_1 \times 10^4 s^{-1}$	40^0	3.18	7.35
$k_1 \times 10^4 s^{-1}$	45^0	5.18	10.12
log A	...	10.80	9.51
ΔE_a^* (k J mol^{-1})	35^0	60.98	55.25
ΔG^* (k J mol^{-1})	35^0	74.63	76.12
ΔH^* (k J mol^{-1})	35^0	71.45	55.52
ΔS^* ($JK^{-1}mol^{-1}$)	35^0	-10.03	-66.82

MECHANISM AND DERIVATION OF RATE LAW

The reaction mechanism involves interaction of $KBrO_3$ with the reactive species of the catalyst to form a complex. The BrO_3^- species has been reported to act as an oxidising agent in acidic as well as in alkaline medium. Pd (II) and Ir(III) chloride has been reported to give a number of possible chloro species dependent on pH of the solution.

Mechanism 1


PdCl2
C1
PdCl+ + Cl-
HBrO3-
k1
k-1
BrO3- + H+
BrO3- +
OH
O
N
H
Paracetamol
k2
k-2
H3C
O-
C
HN
OH
O
Br
O
O
C2
C2 + PdCl+
k3
slow
H3C
O
PdCl+
C
HN
OH
O
Br
O
O
C3
C3 + 2H20
K
Fast
BrO2- +
OH
NH
OH
+ CH3COOH
+ PdCl+
OH
NH
OH
BrO3-
Pd(II)/H+
O
H
N
O
+ H+
N
HO
O
Quinoneoxime

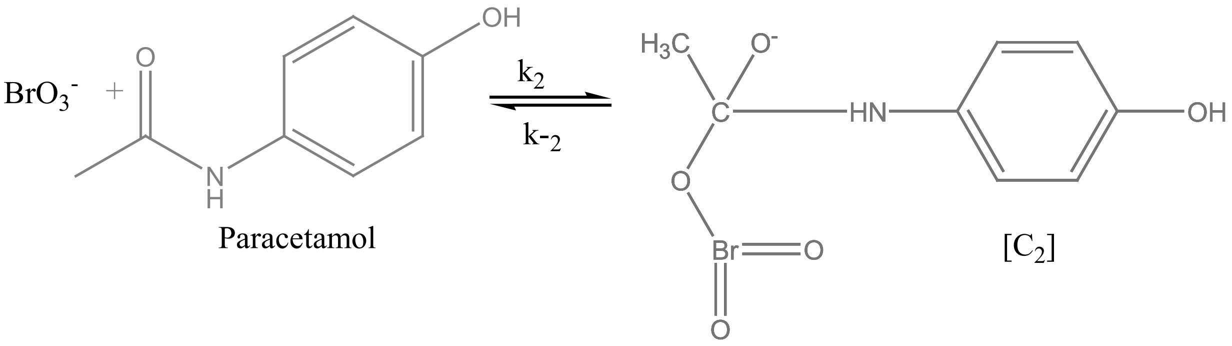
MECHANISM 2

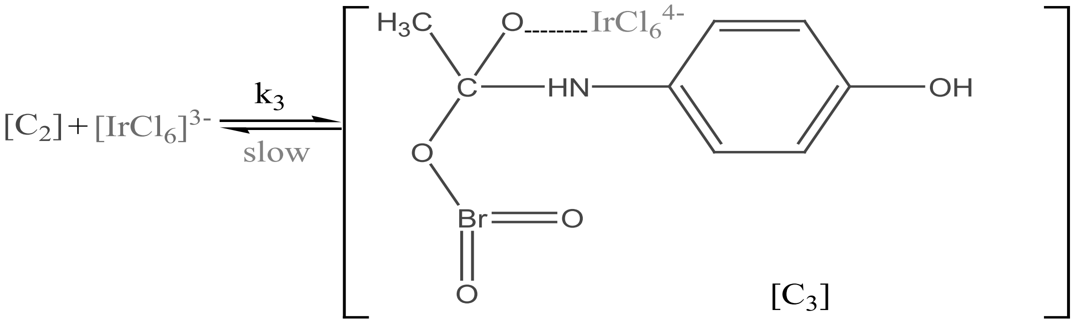
It has been already discussed that $[IrCl_6]^{3-}$is the reactive species of iridium chloride in acidic medium. In view of the reactive species of Ir(III) chloride and $KBrO_3$ and other kinetic features with respect to [Substrate], $[H^+]$, [Hg(II)], $[Cl^-]$ and ionic strength of the medium, the following mechanism steps are proposed. In acidic solution of $KBrO_3$, quick formation of $HBrO_3$ has been reported. Negligible effect of mercuric acetate excludes the possibility of its involvement either as a catalyst or as an oxidant because it does not help the reaction proceed without potassium bromate. Hence the function of mercuric acetate is to act as a scavenger for any $[Br^-]$ ion formed in the reaction. It helps to eliminate the parallel oxidation by Br_2 which would have been formed as a result of interaction between Br^- and bromate ion. Potassium bromate has been used as an oxidant for a variety of compounds in acidic media (Srivastava, S., (1999). sometimes in the presence of a catalyst. In alkaline and acidic medium, potassium bromate is ionised:

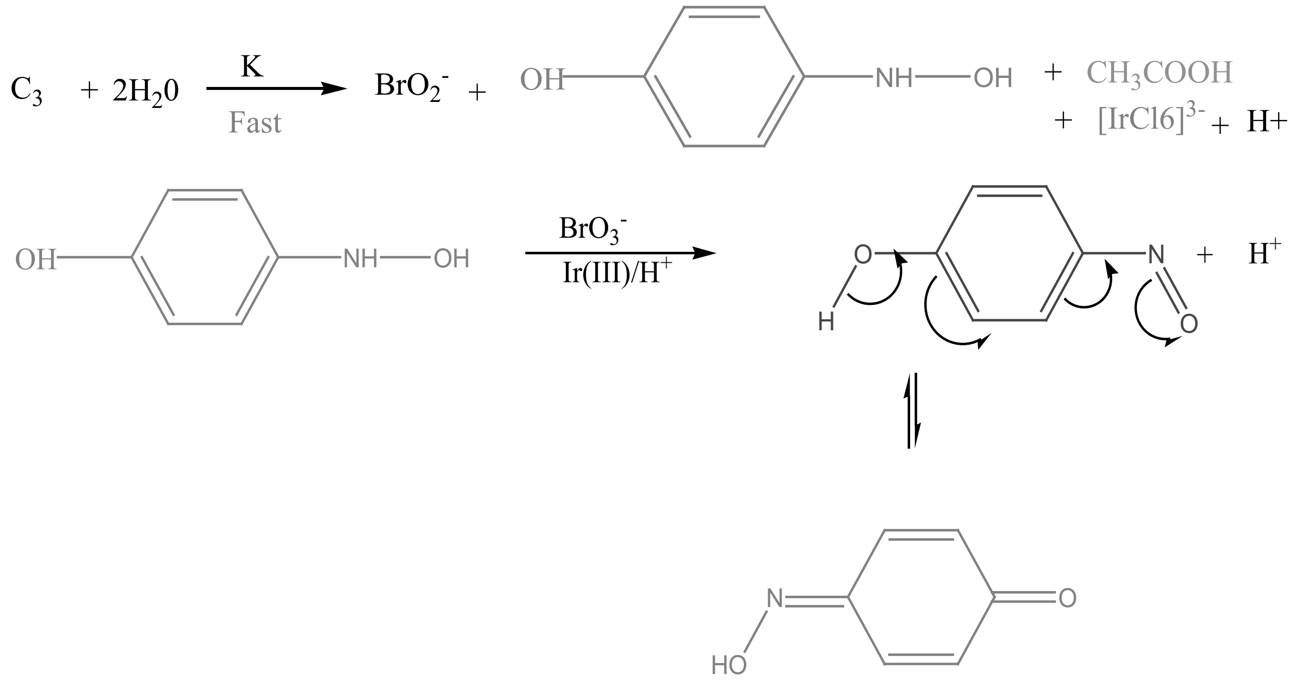
$$KBrO_3\ K^+ + BrO_3^-$$

$$\underset{[C_1]}{[IrCl_5(H_2O)]^{2-}} + Cl^- \rightleftharpoons [IrCl_6]^{3-} + H_2O$$

$$HBrO_3 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} BrO_3^- + H^+$$







Quinoneoxime

Considering the fact that 1 mole of paracetamol is oxidised by 2 mole of bromate for both catalyst Pd(II) and Ir(III) chloride and applying the steady state treatment, with reasonable approximation, the rate law may be written as equation.

$$\mathrm{rate(R)} = \frac{-\mathrm{d}\ [BrO_3]^-}{dt} = 2\mathrm{k}[C_3] \tag{1}$$

On the basis of scheme above step (1) to (4) equation 2-5 can be obtained in the following formes respectively as-

$$R = \frac{2k\ K_1K_2\ K_3\ [Pd(II)]/\ [Ir(III)]\ [PA][HBrO_3]}{[H]^+} \tag{2}$$

At any time in the reaction the total concentration of $HBrO_3$ that is $[HBrO_3]_T$ can be expressed as-

$$[HBrO_3]_T = [HBrO_3] + \ [C_1] + [C_2] + [C_3] \tag{3}$$

Substitution of the variable of $[C_1]$ $[C_2]$ and $[C_3]$ in equation [3]. Equation [4] is obtained.

$$[HBrO_3] = \frac{[HBrO_3]_T}{[H]^+ + K_1 + K_1K_2[PA] + K_1K_2\ k_3\ [Pd(II)]/\ [Ir(III)][PA]} \tag{4}$$

Substituting the value of $[HBrO_3]$ in equation [2] we obtained the expression equation [5].

$$R = \frac{2k\ K_1K_2\ K_3\ [Pd(II)]/[Ir(III)[PA][HBrO_3]_T}{[H]^+ + K_1 + K_1K_2[PA] + K_1K_2\ K_3\ [Pd(II)]/[Ir(III)][PA]} \tag{5}$$

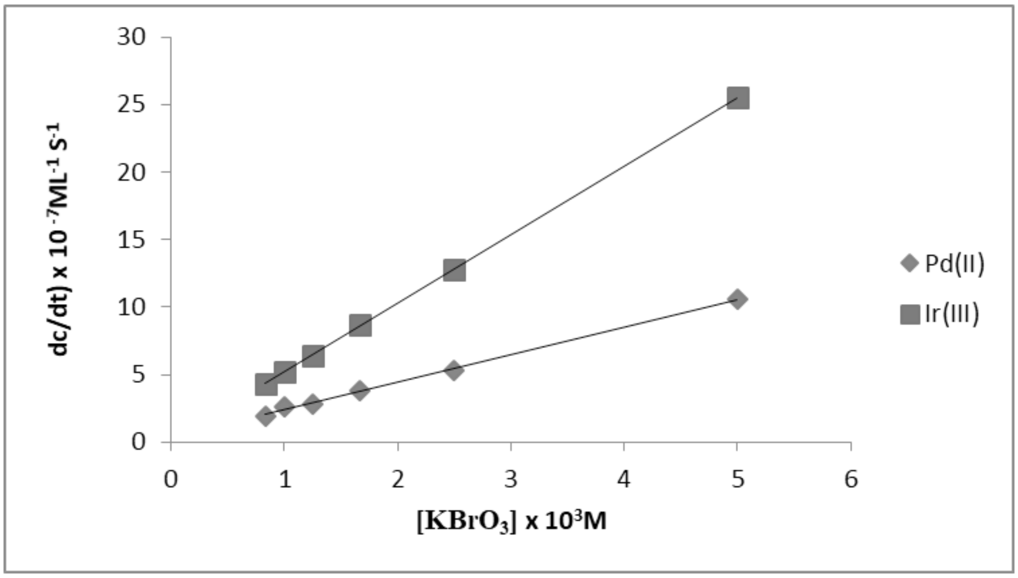


Figure-1: A comparative graph between rate of reaction (-dc/dt) vs [$KBrO_3$] for the oxidation of paracetamol at 35^0C. [$HClO_4$] = 1.00 x 10^{-3}M, [KCl] = 1.00 x 10^{-3} M, [$Hg(OAc)_2$] = 1.25 x 10^{-3} M, Paracetamol [PAM] = 1.00 x 10^{-2} M, Pd(II)/Ir(III) Chloride = 11.2 x 10^{-5} M

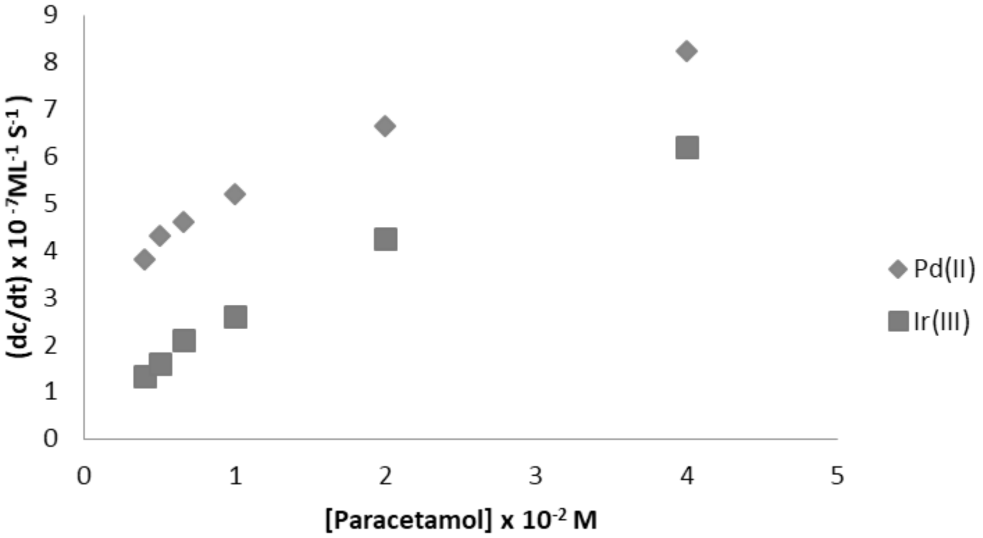


Figure-2: A comparative graph between rate of reaction (-dc/dt) vs [Paracetamol] for the oxidation of paracetamol at 35^0C. [$HClO_4$] = 1.00 x 10^{-3}M, [KCl] = 1.00 x 10^{-3} M, [$Hg(OAc)_2$] = 1.25 x 10^{-3} M, Paracetamol [Ir(III) / Pd(II)] = 11.20 x 10^{-5}M, [$KBrO_3$] = 1.00 x 10^{-3} M.

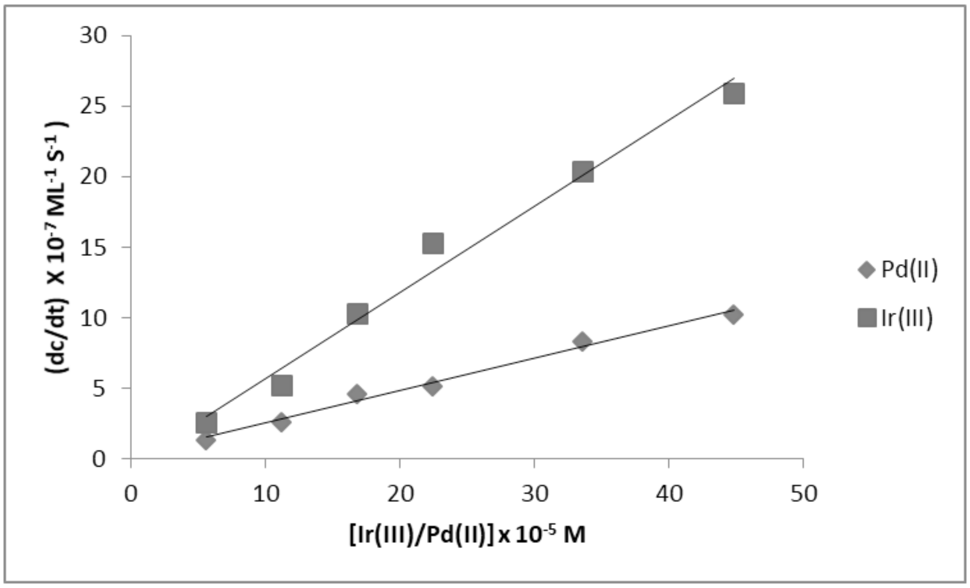


Figure-3: A comparative graph between rate of reaction (-dc/dt) vs [Pd(II)] and [Ir(III)] chloride for the oxidation of paracetamol at 35^0C. [$HClO_4$] = 1.00 x 10 $^{-3}$M, [KCl] = 1.00 x 10 $^{-3}$ M, [$Hg(OAc)_2$] = 1.25 x 10 $^{-3}$ M, Paracetamol [PAM] = 1.00 x 10 $^{-2}$ M, [$KBrO_3$] = 1.00 x 10^{-3} M.

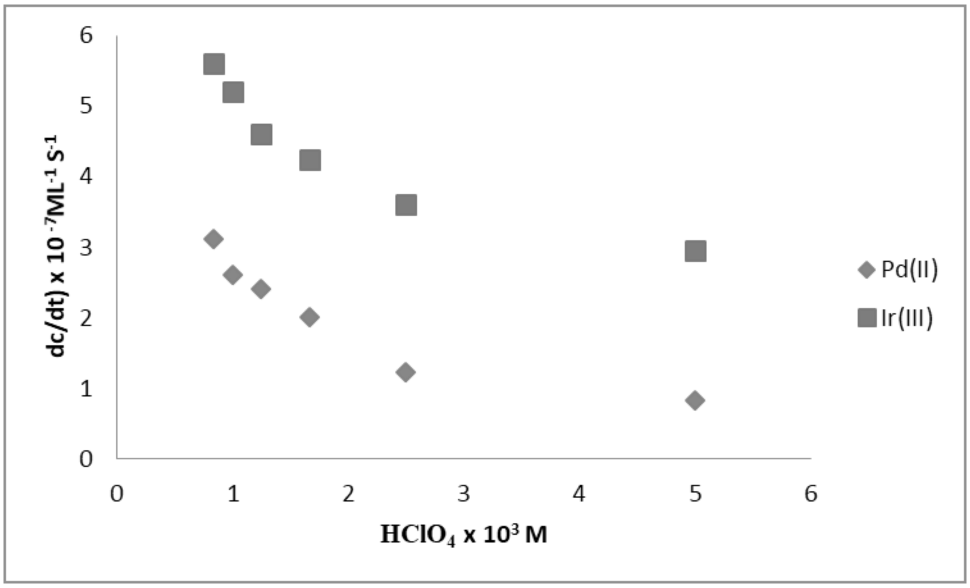


Figure-4: A comparative graph between rate of reaction (-dc/dt) vs [$HClO_4$] for the oxidation of paracetamol at 35^0C. [Ir(III)/ [Pd(II)] = 11.20 x 10^{-5}M, [KCl] = 1.00 x 10 $^{-3}$ M, [$Hg(OAc)_2$] = 1.25 x 10 $^{-3}$ M, Paracetamol [PAM] = 1.00 x 10 $^{-2}$ M, [$KBrO_3$] = 1.00 x 10^{-3} M.

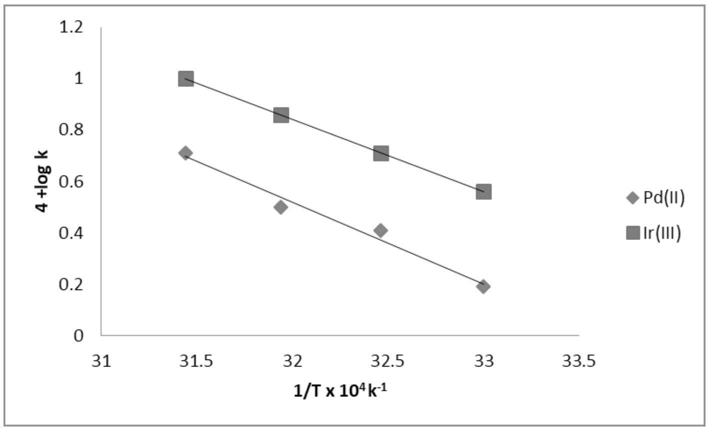


Figure-5: A comparative arrhenius plot of the oxidation of paracetamol on the reaction rate at 35⁰C [Pd(II)/[Ir(III)] Chloride] = 11.2×10^{-5} M, [KCl] = 1.00×10^{-3} M, $[Hg(OAc)_2]$ = 1.25×10^{-3} M [Oxidant $(KBrO_3)$] = 1.00×10^{-3} M, [Paracetamol] = 1.00×10^{-2} M, $[HClO_4]$ = 1.00×10^{-3} M

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FRP-03

DFT by 6-311++G(d,p) (B3LYP) and PED% by Veda-4 Studies of S-benzyl-β-N-(1-(4-fluorophenyl) Ethylidene) Dithiocarbazate

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Abstract—S-benzyl-β-N-(1-(4-fluorophenyl) ethylidene) dithiocarbazate (HL), Schiff base of S-benzyl dithiocarbazate was synthesized by 1:1 condensation between S-benzyl dithiocarbazate and 4-Fluoroacetophenone. The Hard-Soft Schiff base (HL) was characterized by FT-IR, H^1-NMR, Raman, and UV-VIS spectroscopic techniques. Theoretical quantum chemical calculations were performed using DFT in combination with B3LYP exchange correlation functional and 6-311++ G (d, p) basis sets level. The calculated values of chemical potential (μ), HOMO-LUMO energy gap, chemical hardness (η), softness (S), ionization energy (IE), electron affinity (EA), dipole moment (D), electronegativity (χ), electrophilicity (ω) and relative stabilization energy of the compound were 0.30852 eV, 0.15928 eV, -0.1492 eV, 1.5341 eV, -0.22890 eV, -0.07962 eV, 3.4689 Debye, -0.30852 eV, -0.31883 eV and -1624.7264 eV respectively. VEDA-4 (Vibrational energy distribution analysis) software was employed for theoretical FT-IR spectrum analysis which yielded 103 fundamental vibrational modes along with potential energy distribution percentage (PED%) showing non-linearity of HL. Theoretically calculated parameters like H^1-NMR, FT-IR, UV-VIS, Raman, are in good agreement with experimental results. Natural bond orbital analysis (NBO) is performed for HOMO-LUMO, charge delocalization, electrostatic potential and orbital contributions.

Keywords: PED%, Veda, Dithiocarbazate, Electrophilicity, MEP

INTRODUCTION

Dithiocarbazic and its substituted derivatives have received significant consideration over the past few years [1]. Curiosity remains high in these compounds and Schiff bases because of the following reasons: a) dithiocarbazic acid and the Schiff bases derived from them through condensation with various aldehydes and ketones because of the specific geometries of metal complexes [2] and b) the varied distinction in their structures and properties, especially because of their bioactivity [3].The existence of nitrogen and sulphur atoms in the molecular structure of dithiocarbazates [NH2NHCS2] delivers them good capability to coordinate with metal ions and form five-membered chelate rings, yielding metal complexes with interesting structural properties [4]. Their antibacterial [5], antimalarial [6], antiviral [7], antitumor [8,9] and insecticidal [10] effective single-source precursor [11], catalysis [12], photocatalytic production of hydrogen [13], non-linear optical properties [14]. In this contribution we report the synthesis, characterization and DFT studies of bidentate Schiff base derived from the condensation of S-benzyl dithiocarbazate with 4-Fluoroacetophenone.

EXPERIMENTAL

Material and Instrumentation

All the reagents used in the study were of analytical grade and used shorn of supplementary sanitization. Chemicals such as hydrazine hydrate (90%), carbon disulfide and potassium hydroxide were purchased from

Sisco Research Laboratories (SRL) Pvt Ltd and 4-Fluoroacetophenone from Sigma–Aldrich (USA). IR spectra (4000–400 cm^{-1}) were obtained as KBr pellet using a FTIR-8400/8900 Shimadzu spectrophotometer, H^{1}NMR spectra were record on Bruker Ultra shield at 400 MHz, using $CDCl_3$ as a solvent and TMS as internal reference while the UV–VIS absorptions were scanned on a T60 UV–VIS spectrophotometer between 200 and 800 nm using 10^{-5} M solution in acetone and Raman on JYH LABRAM-HR visible (400-1100 nm) spectrophotometer.

Synthesis & Characterization of Schiff Base Ligand (HL)

A hot ethanolic solution (24ml) of 4-Fluoroacetophenoness (1.39 g, 0.01mmol) was added to a hot solution of S-benzyl dithiocarbazate (.396 g, 0.01mmol) in ethanol (26 ml) and the reaction mixture was refluxed on a water bath for 37 mints [15] *see* fig 1. White color needle shaped crystals separated out on cooling which were filtered, washed several times with ethanol, diethyl ether and, subsequently, dried over solid $CaCl_2$ in a desiccator. The product was recrystallized from absolute ethanol when orange color, fibrous crystals were obtained. The synthesized compound was characterized with the aid of different spectral techniques.

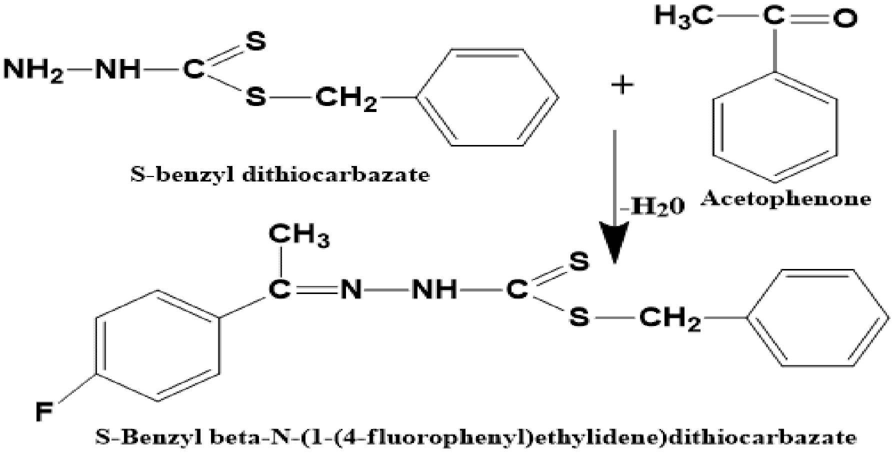


Fig. 1: Experimental Scheme of HL

Yield (2.96 g, 87.83%); m.p. 137^{0}C. Selected IR data (KBr pellet, cm^{-1}): 3437.70ν(N–H), 147.13ν(C–H), 1599ν(C=N), 1283.68 ν(C–F), 1049.91ν(C=S), 698.71 ν(S-C), 1157.75 ν(N–N). *see* fig. 3; ^{1}H NMR (500 MHz, d_6-$CDcl_3$, ppm) δ: 1.80 (s, CH_2), 2.70 (s, 3H, CH_3), 6.97–8.04 (m, 9H, 2ar), 10.47 (s, 1H, NH), *see* fig 2; UV–Vis λmax($CHCl_3$)/nm (log ε): 258 (4.03), 290 (4.26),327 (4.77), 333(4.83), 350 (4.71). *see* fig 8; Raman cm^{-1} 3812.07 ν(N-H), 2832.77 ν(C-H), 1583.67 ν(C=N), 1411.39 ν(C=C), 1295.01 ν(C=S), 1064 ν(N–N) *see* fig 4.

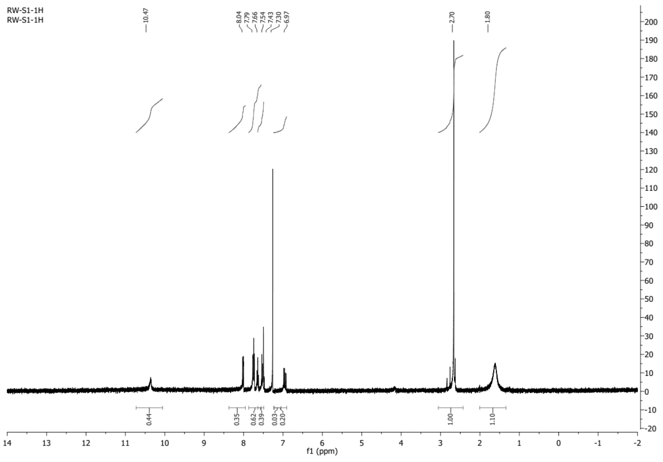


Fig. 2: Experimental Spectra H^{1}NMR of HL^1

DFT STUDIES

The Gaussian 03 program [16] was used for all calculations. Full optimization of all compounds was carried out with density functional theory (DFT) [17] using B3LYP functional [18, 19]. In all calculations, the 6-311++G(d,p) basis set for [20]. Frequency computation was performed to validate the optimization. Infrared vibrational frequencies and the HOMO-LUMO gap for the compound were determined. TD-DFT computations was carried out using the optimized structure in acetone to obtain the electronic spectra of the compounds. In order to obtain natural electron population, natural charge for each atom and frontier molecular orbitals of the compound analysis was performed with natural bond orbital (NBO) code [21]. The electronic absorption spectra and Frontier molecular orbitals of compounds were generated using GaussView-5 [22] and GaussSum [23] software's respectively. Vibrational energy distribution analysis (VEDA-4) programs (author: Michal H. Jamroz) have been employed to investigate 102 simulated vibrational frequency data and to assign prominent vibrations with maximum accuracy see table 1. Geometry optimized structures showed no negative frequencies and were therefore considered as true minima.

RESULTS AND DISCUSSION

FT-IR STUDIES

The experimental and theoretical vibrational frequencies have been precisely allocated and are presented in table 3. Theoretical calculation where done by B3LYP and VEDA 4 program [24-27]. The S-benzyl-β-N-(1-(4-fluorophenyl)ethylidene) dithiocarbazate (HL), consists of 36 atoms and hence 102 vibrational frequency modes are observed. The B3LYP calculation scaled with 0.98 to overcome the theoretical error [28] and experimental and calculated IR-spectra are demonstrated in Fig.3 (a&b).

N-H Vibrations

Generally, ν(NH) stretching vibrations are depicted in the province of 3500-3200 cm^{-1} [29]. The experimental ν(NH) stretching band of HL^1 was observed at 3437.70 cm^{-1} in FT-IR spectrum, however, its theoretical counterpart by B3LYP (6-311++ G (d, P)) level of theory were at 3530cm^{-1}, Ali et al. [30] testified that N-H symmetric stretching vibration of ν(NH) were at 3429 cm^{-1}.

C=N Vibrations

The imperative vibration in HL is C=N (imine linkage) stretching vibration was observed at 1599.73 cm^{-1} However the experimental frequency for C=N has been observed at 1600 cm^{-1}.

C=S Vibrations

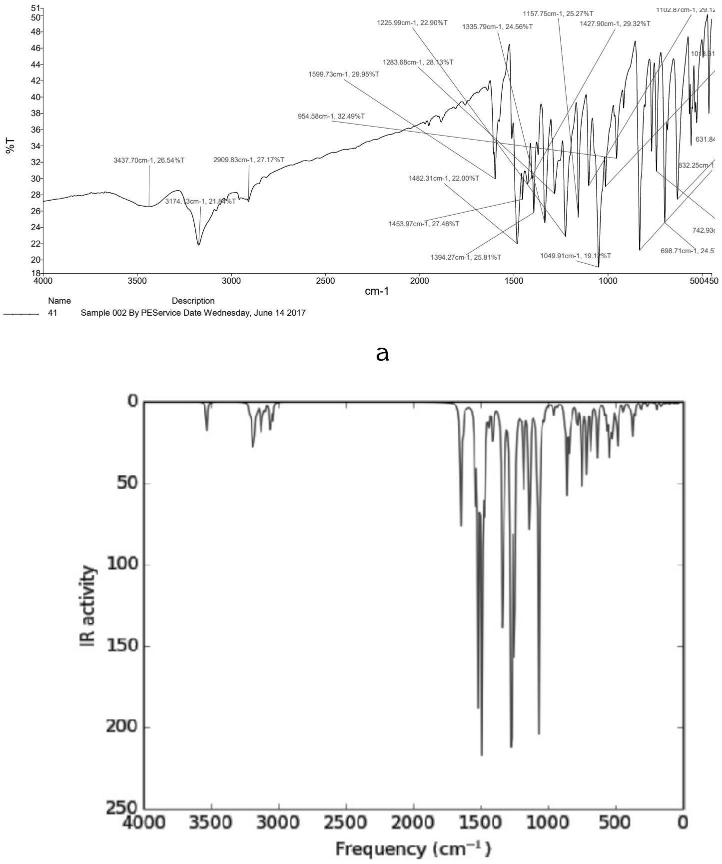
The C=S strong peak for compound HL was observed at 1049.91cm^{-1} in our experimental finding and same by theoretical investigation have strong component at 1066 cm^{-1}.

N-N Vibrations

Usually the N-N vibrations were observed at 1102.87 cm^{-1} in our compound it's found in good agreement with theoretical calculations at 1080 cm^{-1}.

C-F Vibrations

Stretching vibration of C-F is experimentally observed at 1226 cm^{-1} and theoretically at 1221 cm^{-1} by Zierkiewicz et al, in 4-Fluorophenol [31]. However, in our compound experimentally observed at 1283.68 cm^{-1} and theoretically at 1247 cm^{-1}.



a

Fig. 3: Experimental and Theoretical IR spectra of HL (a & b)

Table 1: Comparison of the Experimental (FT-IR) Wavenumbers (cm^{-1}) and Theoretical Wavenumbers (cm^{-1}) of S-Benzyl-β-N-(1-(4-Fluorophenyl)Ethylidene) Dithiocarbazate Calculated by B3LYP level of theory.

Experimental	Calculated(scaled)	Vibrational band Assignments PED (%)
Wave no. in cm^{-1}	wave no. in cm^{-1}	
3437.70	3530	ν_{st}(N10-H22)100
	3207	ν_{st}(C2-H15)98
	3215	ν_{st}(C5-H17)13+ν_{st}(C6-H18)86
	3196	ν_{st}(C5-H17)83+ν_{st}(C6-H18)12
	3192	ν_{st}(C2-H15)94
3147.13	3127	ν_{st}(C8-H19)83+ν_{st}(C8-H20)15
	3114	ν_{st}(C14-H30)99
	3163	ν_{st} (C24-H32)88
	3180	ν_{st}(C24-H32)95
	3172	ν_{st}(C24-H32)92

	3189	ν_{st}(C24-H32)91
	3163	ν_{st}(C25-H33)10
	3154	ν_{st}(C25-H33)85
	3097	ν_{st}(C8-H20)92
	3059	ν_{st}(C14-H30)99
2909.83	3039	ν_{st}(C8-H19)12+ν_{st}(C8-H20)81
	1646	ν_{st}(C5-C6)53+δ(H15-C2-C3)11
	1643	δ(H32-C24-C25)19+δ(C23-C28-C27)+ν_{st}(C24-C25)64
	1629	ν_{st}(C4-C5)59
	1623	ν_{st}(C23-C28)66
1599.73	1600	ν_{st}(N9-C7)57
	1539	ν_{st}(C1-C2)10+δ(C2-C3-C4)12+δ(H15-C2-C3)47
	1526	ν_{st}(C23-C28)11+δ(H32-C24-C25)58+δ(C24-C25-C26)12
	1515	δ(H22-N10-N9)26+δ(H19-C8-H21)35
	1490	δ(H22-N10-N9)32+δ(H19-C8-H21)30
1482.31	1484	ν_{st}(C23-C28)27+δ(H34-C26-C27)46
	1472	δH19-C8-H20)67
1453.97	1467	δ(H31-C14-H30)51+τ(H30-C14-S13-C11)37
1427.90	1437	ν_{st}(C1-C2)35+δ(H15-C2-C3)29
1394.27	1407	δ(H19-C8-H20)79
	1361	δ(H32-C24-C25)88
	1340	ν_{st}(C23-C28)70+δ(H30-C14-S13)13
1335.79	1337	ν_{st}(C1-C7)43
	1332	ν_{st}(C1-C2)60
	1323	δ(H18-C6-C1)69
	1279	δ(H31-C14-H30)33+τ(H30-C14-S13-C11)45
	1270	ν_{st}(N10-C11)61
1283.68	1247	ν_{st}(F29-C4)55+δ(H15-C2-C3)16
1225.99	1225	ν_{st}(C14-C23)40+δ(H32-C24-C25)16+δ(C23-C28-C27)10

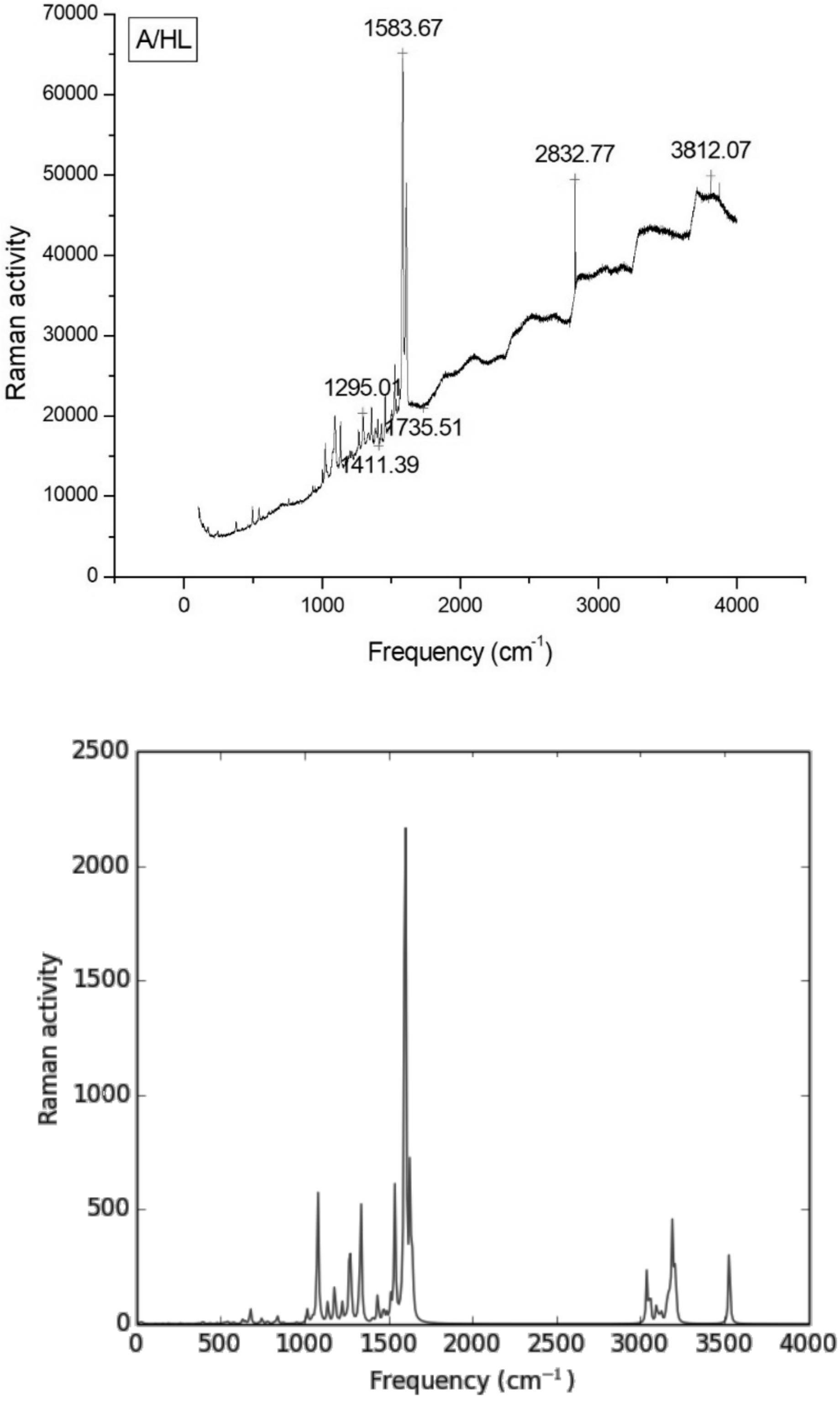
	1204	ν_{st}(C24-C25)21+δ(H32-C24-C25)74
	1186	ν_{st}(C23-C28)12+τ(H31-C14-S13-C11)11+δ(H30-C14-S13)64
	1181	δ(H30-C14-S13)48+ν_{st}(C23-C28)14+δ(H15-C2-C3)52
	1180	ν_{st}(C5-C6)11+ν_{st}(C1-C2)10+δ(H30-C14-S13)12
1157.75	1140	ν_{st}(N9-N10)44
	1130	ν_{st}(C1-C2)15+δ(H15-C2-C3)54
	1101	ν_{st}(C23-C28)40+δ(H34-C26-C27)31
1102.87	1080	ν_{st}(N9-N10)15+τ(H20-C8-C7-C1)26
1049.91	1066	ν_{st}(S12-C11)48+δ(C11-N10-N9)13
	1050	ν_{st}(C24-C25)36+δ(C24-C25-C26)33+δ(H32-C24-C25)20
	1040	τ(H19-C8-C7-C1)63+δ(H19-C8-H20)10
	1028	δ(H15-C2-C3)13+δ(C2-C3-C4)67
1013.61	1017	δ(C24-C25-C26)44+ν_{st}(C24-C25)42
	1001	τ(H32-C24-C25-C26)72+σ(C14-C24-C28-C23)10
	993	τ(C2-C3-C4-C5)12+τ(H32-C24-C25-C26)83
	986	τ(H32-C24-C25-C26)76+τ(C23-C28-C27-C26)10+ τ(C24-C25-C26-C27)10
954.58	956	τ(H20-C8-C7-C1)20+ν_{st}(C7-C8)28
	951	τ(H15-C2-C3-C4)67+τ(C1-C2-C3-C4)17
	875	δ(H30-C14-S13)15+τ(H31-C14-S13-C11)43
	858	τ(H15-C2-C3-C4)81
	855	τ(H32-C24-C25-C26)94
832.25	840	ν_{st}(C3-C4)69
	824	τ(H15-C2-C3-C4)94
	821	δ(C25-C26-C27)41+ν_{st}(C14-C23)25
	781	τ(C23-C28-C27-C26)10+τ(H34-C26-C27-C28)29+ τ(H32-C24-C25-C26)10
742.93	748	ν_{st}(C7-C8)22+δ(C7-N9-N10)12
	731	τ(C1-C2-C3-C4)59+τ(H15-C2-C3-C4)13+τ(C1-C7-N9-

		N10)10
	712	τ(C23-C28-C27-C26)33+τ(H34-C26-C27-C28)56
698.71	679	ν_{st}(S13-C14)57
	649	δ(C1-C2-C3)15+ν_{st}(C4-C5)10+δ(C2-C3-C4)61
	636	δ(C24-C25-C26)65+δ(C23-C28-C27)11
631.84	632	δ(C24-C25-C26)14+ν_{st}(S12-C11)26
	582	τ(H22-N10-N9-C7)55
	578	σ(C14-C24-C28-C23)10+δ(C25-C26-C27)20+ δ(C23-C28-C27)13+δ(S13-C14-C23)12
	561	ν_{st}(S12-C11)11+δ(C1-C7-N9)21
	545	σ(S12-N10-S13-C11)68
	533	δ(C11-N10-N9)40
	518	τ(C2-C3-C4-C5)65
	481	σ(C14-C24-C28-C23)46
	439	δ(C1-C2-C3)10+δ(C2-C1-C7)53
	424	τ(H17-C5-C6-C1)76+τ(C2-C3-C4-C5)66
	413	τ(H32-C24-C25-C26)18+τ(C24-C25-C26-C27)75
	397	ν_{st}(S12-C11)19+δ(C1-C7-N9)61
	385	τ(C2-C3-C4-C5)11+τ(C1-C7-N9-N10)53
	370	δ(C2-C3-C4)11+δ(C7-N9-N10)32
	354	δ(C11-S13-C14)58+τ(H31-C14-S13-C11)17
	307	δ(C2-C1-C7)46
	262	τ(C1-C7-N9-N10)72

ν-stretching: δ-bending: τ-torsional: σ-out of plane.

RAMAN SPECTRA ANALYSIS

The HL Schiff Base is also scrutinized by both experimental (JYH LABRAM-HR visible (400-1100 nm) spectrophotometer) and theoretical simulation (Gaussian 03 package) by using B3LYP/ 6-311G ++ (d, p) basis set demonstrated in Fig 4 (a&b) with few significant peaks like νC=N→(1619.53cm^{-1}) =(1636.02cm^{-1}), νC=S→(1295.01cm^{-1})=(1273.23cm^{-1}), νC-H→(2832.77 cm^{-1})=(3194.36cm^{-1}), and ν(N-H)→(3812.07 cm^{-1})=(3542.41cm^{-1}, νC-F→(1226.32 cm^{-1})= (1273.76cm^{-1}) are clearly observed in the theoretical Raman spectra see fig 4(A&B).



B

Fig. 4: Experimental and Theoretical IR spectra of HL (A & B)

UV-VIS SPECTRAL ANALYSIS

S-Benzyl-β-N-(1-(4-fluorophenyl)ethylidene)dithiocarbazate (HL) was theoretically as well as experimentally investigated for electronic spectra in acetone by TD-DFT/B3LYP/6-311G++(d,p) level of basis set in Gaussian 03 package. The transitions between inter frontier orbitals for wavelengths corresponding to maximum oscillator strength of simulated results with contemporary experimental observations are presented in Table 2 and in Fig. 5 (A&B).

Table 2: The Experimental and Computed Wavelength (nm), Absorbance and Oscillator Strengths(f) of HL in Acetone Solution.

Excitation	Singlet A	E(eV)	Wavelength(nm)			Oscillator Strength	Assignments	Transition
			Ex	Abs	Cal			
Excited-82→84 82→85	0.66889 0.13137	3.3994	393.2	3.443	398.96	0.0003	n→π* π→π*	H-1→L H-1→L+1
Excited-1 81→84 83→84	0.12649 0.63833	3.6972	400.4	3.672	335.35	0.9199	n→π* n→π*	H-2→L H→L
Excited-1 81→84 83→84	0.66598 -0.11981	4.0065	321.23	3.299	309.46	0.0623	π→π* n→π*	H-2→L H→L

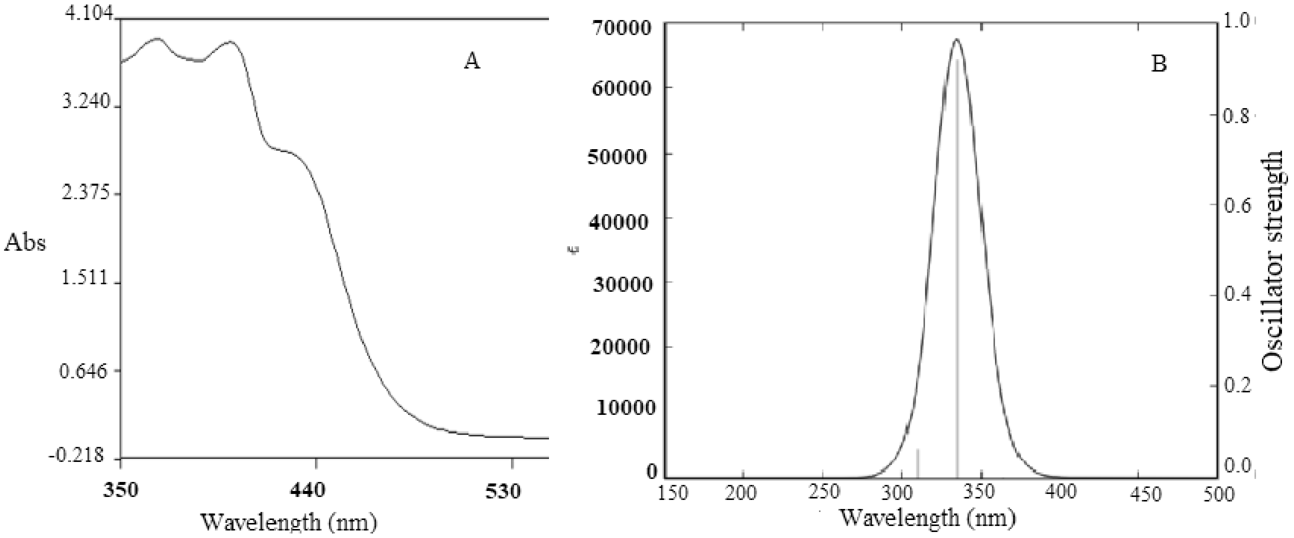


Fig. 5 (A&B): Experimental & Theoretical UV-Spectra of S-Benzyl-β-N-(1-(4-fluorophenyl) ethylidene) dithiocarbazate in acetone solution.

OPTIMIZED GEOMETRY

The optimized structure has been shown in Fig. 6 and the geometrical parameters such as bond length, bond angle and dihedral angle have been tabulated in Table 3. It is evident that if dihedral angles allied with 4-adajacently bonded atoms are approximately equal to 0^0 or 180^0, it infers that accompanying atoms lie virtually in same plane. Keeping this point under contemplation, the entire molecular geometry of HL is allied along three planes-plane-I, II and III. All the atoms of the phenyl ring of benzyl moiety of the HL lie in plane-I, having average bond length associated with C=C in benzene ring was 1.36 A^{o}. Dithio moiety belongs to plane II and remaining portion comprises to plane III revealed by calculated dihedral angles that plane-I and II are inclined at 90 A^{0} and plane-II and III are inclined at acute angle 30 A^{0} of HL respectively.

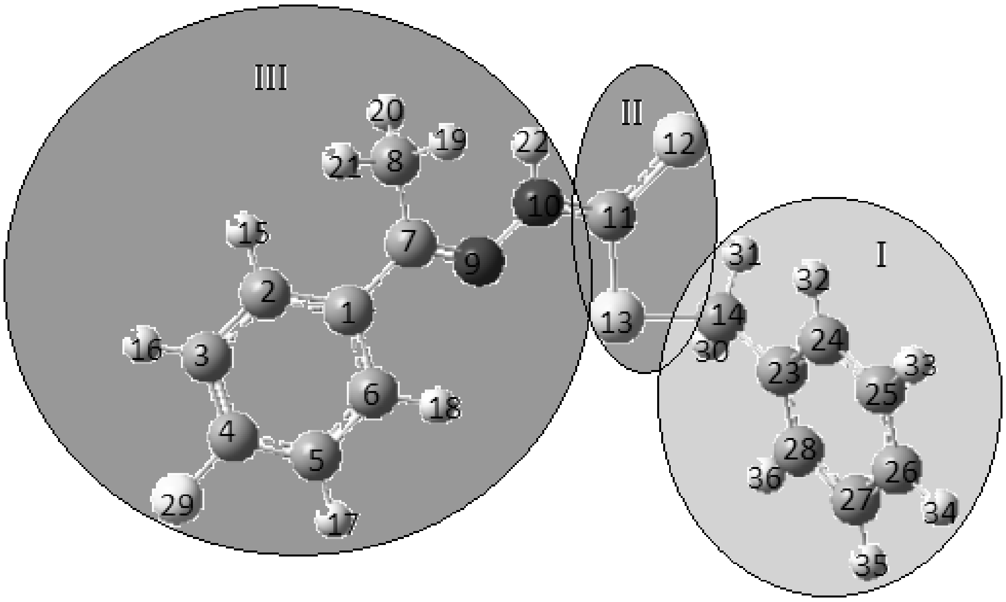


Fig. 6: Optimized structure of S-Benzyl-β-N-(1-(4-fluorophenyl)ethylidene)dithiocarbazate (HL) with planar differentiation (different colours signifies different planes).

Table 3: Calculated bond Lengths, bond Angles and Dihedral Angles of S-Benzyl-β-N-(1-(4-Fluorophenyl)Ethylidene) Dithiocarbazate

Bond-length (in Å)	Bond-Angle (in ^{0})	Dihedral Angle (in ^{0})
C3-C2=1.540	C14-C23-C24=120.00	C3-C2=C1-C7=-180.00
C3=C4=1.355	C23=C28-C27=120.00	C2=C1-C7=N9=180.00
C14-C23=1.54	C11-S13-C14=109.47	C1-C7=N9-N10=-180.00
S13-C4=1.780	N10-C11-S12=120.00	C8-C7=N9-N10=0.000
C11-S13=1.780	S12=C11-S13=120.00	C7=N9=N10-C11=-150.00
C11=S12=1.566	N9-N10-C11=109.471	N9-N10-C11=S12=150.00
N10=C11=1.470	N10-C11-S13=120.00	N9-N10-C11-S13=-30.00
N9-N10=1.400	C7=N9-N10=120.00	N10-C11-S13-C14=-150.00
C7-N9=1.293	C8-C7-N9=120.00	S12=C11-C13-C14=30.00
C7-C8=1.540	C1-C7-N9=120.00	C11-S13-C14-C23=60.00
C1-C7=1.540	C1-C7-C8=120.00	S13-C14-C23-C28=90.00

NBO ANALYSIS

The calculated bonding orbital with maximum electron density (occupancy) is called natural bond orbital (NBO). The sequence of natural localized orbital sets include.

(Atomic orbitals) → natural atomic orbitals (NAOs) → hybrid orbitals (NHOs) → bond orbitals (NBOs) → (semi-)localized molecular orbitals (NLMOs) →(Molecular orbital)……(a)

The NBO analysis programme with host programme works in tandem, that performs the wave function calculation to be analysed. The sturdiest interaction of stabilization between dominant donors (i) and acceptors (j) is due to stabilization of orbital interaction which is proportional to the energy difference between interacting orbitals. Quantitatively in NBO basis the interactions are expressed by means of second order perturbation interaction energy E(2) between bonding and antibonding orbital see table 5. This energy also portrays an evaluation of the off diagonal NBO fock matrix element and are determined by succeeding mathematical formula.

$$E^{(2)} = \Delta Ei,j = \mathrm{qi}\frac{(\mathrm{Fi,j})^2}{\varepsilon\mathrm{i} - \varepsilon\mathrm{j}}$$

Where F(i, j) is off diagonal, qi is donor orbital occupancy, εi and εj are diagonal elements (orbitalenergy) of Fock matrix.

Table 5: Second order Perturbation theory Analysis of fock Matrix in NBO basis for larger E (2) value.

Donor	Acceptor	E(2) [kcal/ mol]	E(j)- E(i) [a.u.]	F(i, j) [a.u.]	Donor	Acceptor	E(2) [kcal/ mol]	E(j)- E(i) [a.u]	F(i, j) [a.u]
πC1-C2	π*C3-C4	19.16	0.27	0.065	LP(1)N9	π*C7-C8	10.94	0.78	0.083
	π*C5-C6	20.11	0.29	0.069	LP (1)N10	π*C7-N9	27.46	0.29	0.083
	π*C7-N9	16.42	0.27	0.061		π*C11-S12	67.66	0.21	0.109
πC3-C4	π*C1-C2	21.04	0.30	0.071	LP(2) S12	σ*C10-C11	11.37	0.63	0.078
	π*C5-C6	17.13	0.30	0.065	LP (2) S13	π*C11-S12	42.17	0.16	0.078
πC5-C6	π*C1-C2	17.81	0.28	0.064	LP (3) F14	π*C3-C4	18.14	0.43	0.086
	π*C3-C4	23.57	0.28	0.073	LP (2) S12	π*C11-C13	15.10	0.38	0.009
πC24-C25	π*C23-C28	20.97	0.28	0.069	π*C3-C4	π*C5-C6	235.78	0.01	0.082
	π*C26-C27	20.44	0.28	0.068	π*C7-N9	π*C1-C2	123.17	0.01	0.064
πC26-C27	π*C23-C28	19.89	0.28	0.068	πC23-C28	π*C24-C25	19.40	0.29	0.067
	π*C24-C25	19.77	0.29	0.067		π*C26-C27	20.57	0.28	0.068

E(2) means energy of hyper conjugative interaction (stabilization energy).
E(j)-E(i) is the energy difference between donor(i) and acceptor (j) NBO orbitals.
F(i,j) is the Fock matrix element between i and j NBO orbitals

MOLECULAR ELECTROSTATIC POTENTIAL

The molecular electrostatic potential (MEP) maps or molecular electrical potential surfaces or electrostatic potential energy maps are accountable for the chemical behavior like chemical bonding, electronegativity etc of molecular system and these maps are created by nuclei and electrons at specific point. Region with low potential or region with higher than average electrostatic potential energy has strong influence of positively charged particles and vice versa and their biological activity recognition as well as reactivity towards positive and negative charged regions can be forecasted through pictorial illustration by quantum-chemical simulations and different regions may be color coded specifically (Fig 7). The substantial positive potential and electron deficient coded in the form of light blue color lie mainly on the terminated hydrogen atoms attached to N, CH_3, CH_2 and benzene carbon atoms, however, the S, N and C atoms having yellow and green color are under intermediary potential regime.

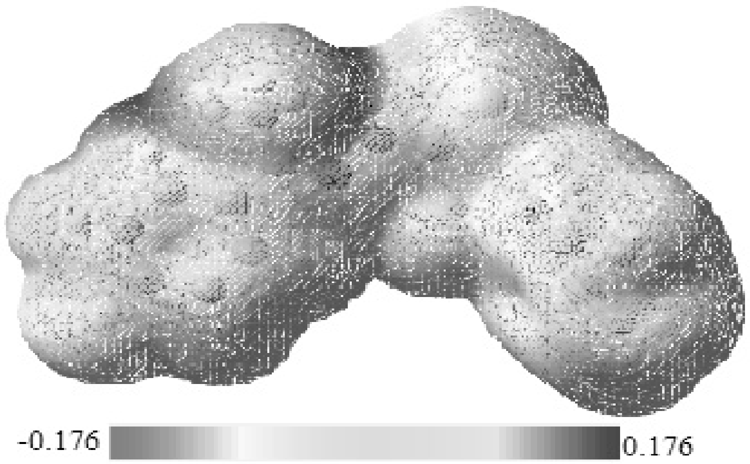


Fig. 7: Electrostatic potential of S-Benzyl-β-N-(1-(4-fluorophenyl)ethylidene)dithiocarbazate (HL) mapped into electron density isosurface (0.020 e/Å3).

FRONTIER MOLECULAR ORBITALS

Frontier molecular orbitals have been shown in fig. 8. Small inter frontier orbitals of a molecule are chemically more active and has low kinetic stability [32-36] among the frontier molecular orbitals. The biological effectiveness of molecular system is determined from electrophilic and low energetic, highest occupied molecular orbital (HOMO) which corresponds to ionization potential(I). Nucleophilic and high energetic, lowest unoccupied molecular orbital (LUMO) corresponds to electron affinity (electron gain enthalpy) (A) [37]. Electrophilicity, global hardness(η) and chemical potential(μ) describes the potency of the molecule and which are expressed in terms of $A = -E_{LUMO}$ and $I = -E_{HOMO}$. Chemical potential and hardness are derived by mathematical expression; $\mu = (I + A)/2$ and $\mu = (I - A)/2$ 0.30852 eV and -0.1492 eV respectively.

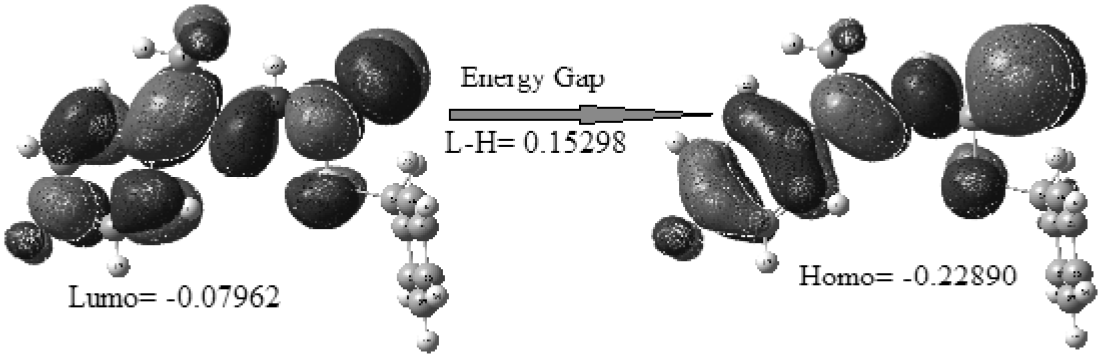


Fig. 8: Frontier molecular orbitals of S-Benzyl-β-N-(1-(4-fluorophenyl)ethylidene)dithiocarbazate (HL)

CONCLUSION

The (HL) ligand was obtained by condensation of S-benzyl dithiocarbazate with 4-Fluoroacetophenone and the synthesized compound was characterized by FT-IR, UV-VIS, ^1H NMR, and Raman. The projected structure of Schiff base was geometrically optimized and their structural parameters were calculated by DFT with B3LYP exchange correlation functional in combination with 6-311++G (d, p) basis sets using Gaussian 03 package.

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Effect of Potassium and Phosphorus Fertilization on Green Herb Yield of some Medicinal Plants of Himalaya Region *(UTTARAKHAND)* INDIA

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Abstract—Origanum vulgare (oregano) and Thymus serpyllem (wild thyme) is a member of the Lamiaceae family and is an indigenous aromatic and medicinal plant of Europe and Asia(Mediterranean region). At present, it is cultivated the mild, temperate climates of in North America, Europe, Asia, North Africa, and America in a large scale due to its economic importance. However, studies on agronomic factors such as application of potassium humate and irrigation intervals as well as nitrogen fertilization on yield and essential oils of oregano have not been investigated thoroughly until now. The observation on plant growth, yield per hectare, leaf area index, rhizome yield will be recorded. Profit would be examined and production will be popularized among local youth. it is commercially grown. The objective of this study was to examine the effects of different level of N, P and K on green herb yield and some herb chemical constituents (N, P, K) in order to recommend a reliable nutrient management for commercial growers. Results showed that, yield generally increase in accordance with the increases in N, P and K fertilizer rates.

Keywords: Nitrogen(N) Potassium (K), phosphorus (P), Oregano (Origanum vulgare). Thyme (thymus serpyllem)

INTRODUCTION

Thymus serpyllem L. which is an aromatic and medicinal plant indigenous to Europe and Asia is a member of the Lamiaceae family. *T. serpyllum*, known as wild thyme, is native to Mediterranean Europe and North Africa, mainly at the higher altitudes. Wild thyme is a creeping dwarf evergreen shrub with woody stems and a taproot. It forms matlike plants that root from the nodes of the squarish, limp stems. The leaves are in opposite pairs, nearly stalkless, with linear elliptic round-tipped blades and untoothed margins. The plant sends up erect flowering shoots in summer. The usually pink or mauve flowers have a tube-like calyx and an irregular straight-tubed, hairy corolla. The upper petal is notched and the lower one is larger than the two lateral petals and has three flattened lobes which form a lip. Each flower has four projecting stamens and two fused carpels. The fruit is a dry, four-chambered schizocarp. Brecked thyme is dwarf shrub that has a stong fragrance and forms mat-like stands, and the base of its stems gets woody as it ages. Its habitat is limited to countries around the Baltic Sea, although it has made extensive inroads into continental Russia. Breckland thyme is the northernmost species in its large genus. It has a very important source of nutrition for large blue and eastern baton blue butterfly caterpillars because they only lay their eggs in Breckland thyme flowers and they only eat thymeHoneybees like the nectar , making it a good honey plant. Creeping and mounding variants of *T. serpyllum* are used as border plants and ground cover around gardens and stone paths. It may also be used to replace a bluegrass lawn to xeriscape low to moderate foot traffic areas due to its tolerance for low water and poor soils. The objective of this study was to recommend a reliable nutrient management for commercial wild thyme growers by examining the effects of different rates of P and K fertilizations on green herb yield (leaf+ stalk + flower) and some herb nutrients (N, P, K). *Origanum vulgare*) is a flowering plant in the mint family (Lamiaceae). It is native to temperate Western and Southwestern Eurasia and the Mediterranean region. Oregano is a perennial herb, growing from 20–80 cm (7.9–31.5 in) tall, with opposite leaves 1–4 cm (0.39–1.57 in) long. The flowers are purple, 3–4 mm (0.12–0.16 in) long, produced in erect spikes. It is sometimes called wild marjoram, and its close relative, O. majorana, is known as sweet marjoram. Oregano contains essential oils, rich in the two isomeric phenols carvacrol and thymol (Fleisher and Sneer, 1982; Kokkini and Vokou, 1989 and Vokou *et al.,* 1993). The use of oregano as a medicinal plant is attributed to the biological properties of the herb and its essential oil composition. The objective of this study was to recommend a reliable nutrient management for commercial wild thyme growers by examining the effects of different rates of N, P and K fertilizations on green herb yield (leaf + stalk + fl.

MATERIALS AND METHODS

Small size plant will be selected for cultivation. The net plot size will be kept at 1.34*1.00m. twenty seven treatment combinations of fertilizers would be consisted with three levels nitrogen (0,76,145 kg./ha.). Three levels of phosphorus (0,126,252 kg./ha.) and three level of potassium (0,76,151 kg./ha.). The hole quantity of phosphorus half of potash and nitrogen was applied at the time of planting the rest half dose of nitrogen and potash was given one month after planting. The observation on plant growth, yield per hectare, leaf area index, rhizome yield will be recorded. Profit would be examined and production will be popularized among local youth. Experiment plot would be selected on Pithoragarh, Uttrakhand. Green herb yields were found generally higher in the second year of the experiment in all of the treatments. Each year, yield response to the enhanced, K and P fertilizations were found positive and statistically significant at 2% level. The interaction effect of N, P and K fertilizations on yield was not found significant in the first year where as was determined significant in the second year (Table 2). In this context, the highest yield was obtained in the highest rate of N (151 Kg urea / ha.) P (126 kg phosphorus/ha.) and K (151 kg potash/ha.) fertilizations. Nutrient elements (N, P and K) of the green herb were also analyzed in both of the study years. Results of the statistical analyses showed that the herb N, P and K contents were significantly higher. On the other hand, in the first and second years of this study, statistically significant interaction effects of N, P and K fertilizations were determined on the N, P and k contents of the herb respectively.

The data of this study showed that N ,P and K fertilizations positively affect the developments in *Origanum vulgare* , its yield as well as its quality as a medicinal and herbaceous plant. Among many plant growth factors, the nutritional requirements of the crops are considered to be the most important factor. Generally the growth, development, yield and the quality of herbs are affected by genetic background; Phosphorus also has many other cellular functions in plants and affects the primary and secondary metabolites. Therefore, P fertilization in medicinal herbs is strongly recommended especially in cites with low available soil .

RESULTS AND DISCUSSION

Green herb yields were found generallyhigher in the second year of the experimentin all of the treatments. Each year, yield response to the enhanced,. The interaction effect of N, P and K fertilizations on yield was not found significant in the first year where as was determined significant in the second year (Table 2). the highest yield was obtained in the highest rate of N (151 Kg urea /ha.) P (125 kg phosphorus/ha.) and K (150 kg potash/ha.) fertilizations. Nutrient elements (N, P and K) of the green herb were also analyzed in both of the study years. in the first and second years of this study, statistically significant interaction effects of N, P and K fertilizations were determined on the N, P and k contents of the herb respectively. The data of this study showed that N ,P and K fertilizations positively affect the developments in *Origanum vulgare* and *Thymus serphyllum* , its yield as well as its quality as a medicinal and herbaceous plant. Among many plant growth factors, the nutritional requirements of the crops are considered to be the most important factor.

Table.1: Soil Properties of Experimental Site

Site	Colour (dry)	elevation	Soil text	Particle-size distribution(%)			Ph (1:2.5)	Org carbon Kg-1	Cec Cmo (p+) Kg-1
				Sand (2.0-0.05 mm)	silt (0.05-0.002 mm	Clay (<0.002 mm)			
L.S.M.G.P.G.C. Pithoragarh	Olive yellow	1498	silt	7.6	68.9	23.5	5.9	14.7	9.3

Table.2 : Effect of N, K and P Fertilization on Green Herb Yield (kg/ha.) for 2012 and 2013 Seasons

Combination no.	First season (2011)	Second season (2012
	Thymus serphyllum((Origanum vulgare)	Thymus serphyllum(Origanum vulgare)
C1	15400(14500)	16700(17700)
C2	15000(15000)	17300(18400)
C3	16400(15600)	18500(18800)
C4	16000(15000)	19700(19100)
Mean	16240 (15340)	18140(18500)

C1=control,C2=N:151(151)kg/ha.)+P:126(250)kg/ha.+K75(75kg/ha),C3=N75(75kg/ha.)+P:250(0 kg/ha.)+K :75(75 kg/ha.) and C4=N:150(150 kg/ha.)+P :250(125kg/ha.)+K:150(150 kg/ha.)

Table.3: Effect of N, P And K Fertilization on N, P and K Conent (%) For2011 and 2012 Seasons.

Combination no.	%					
	N		P		K	
	Thymus serphyllum((Origanum vulgare)		Thymus serphyllum((Origanum vulgare)		Thymus serphyllum((Origanum vulgare)	
	First season (2012)	Second season (2013)	First season (2012)	Second season (2013)	First season (2012)	Second season (2013)
C1	1.824(1.085)	1.824(1.086)	0.251(0.173)	0.251(0.173)	1.071(0.685)	1.071(0.685)
C2	1.827(1.240)	1.820(1.264)	0.257(0.177)	0.267(0.170)	1.130(0.680)	1.164(0.691)
C3	1.820(1.152)	1.831(1.182)	0.251(0.184)	0.251(0.180)	1.170(0.600)	1.180(0.703)
C4	1.832(1.500)	1.836(1.524)	0.261(0.194)	0.271(0.100)	1.100(0.707)	1.224(0.700)
Mean	1.828(1.240)	1.830(1.264)	0.255(0.182)	0.260(0.185)	1.147(0.695)	1.162(0.695)

C1=control,C2=N:150(150)kg/ha.+P:126(250)kg/ha.)+K:75(75)kg/ha,C3=N76(75kg/ha.)+P:250(250kg/ha.)+K:76(75 kg/ha.) and C4=N:151(150 kg/ha.)+P :126(125kg/ha.)+K:151(150 kg/ha.).

The data of this study showed that N, P and K fertilizations positively affect the developments in *T.sepyllem* and *Origanum vulgare* , its yield as well as its quality as a medicinal and herbaceous plant. Potassium fertilizers proved its role in plant metabolism, carbohydrate synthesis, water transport in xylem, cell elongation. Singh (2001) reported that addition of K resulted with higher herb yields. In this current study, green herb yield, some of the herb nutrient elements like N, P, K positively responded toN, P and K fertilizer treatments. The highest herbal yield was determined in 150 kg urea/ ha.+1 25 kg phosphorus/ ha.+150 kg potash/ha. treatment in both of the study seasons. The present study can be concluded that if the herb yield evaluated and weighed and ranked according to the treatments . In case N fertilization is necessary according to soil testing, recommendations should be followed.

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FRP-05

Characterization of Activated Bagasse Fly Ash (ABFA) For Sugar Decolorization

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Abstract—Bagasse fly ash (BFA), a waste material generated in the sugar industry, collected from a local sugar factory, was used as a low cost and effective adsorbing surface for the removal of colourants from aqueous sugar solution. The raw material employed for the production of the new adsorbent is widely available across the world free of cost. The Physical (bulk density, hardness) and chemical properties (pH, conductivity, ash) of the activated BFA samples were analyzed using standard methods. Batch studies were performed to evaluate the adsorption capacity was followed as a function of pH, adsorbent dose, effect of ionic strength, shaking time, concentration of adsorbate and temperature. Under the optimum conditions used, more than 90% of the colourants under study were successfully removed. Relative efficiency of decolorization was compared with the commercial activated carbon (Darco Carbon) and ion exchange resin. It was found that the BFA showed the satisfactory physical and chemical properties. The decolorizing property was much better than the commercial carbon making it a good decolourizer in the sugar refinery/industry.

INTRODUCTION

One of the low-cost adsorbents, BFA is a waste material obtained from the particular collection devices attached to the flue gas line of the sugar cane bagasse-fired boilers. BFA has good adsorption properties for organics, heavy metals and sugar colourants removal and is, therefore, used as an adsorbent in the treatment of industrial waste water[1,2] and sugar decolourization[3]. The literature mentions many precursors for activated carbon such as bagasse[4] rice husk[5] rice bran[6] etc. Sugar cane bagasse is a byproduct of sugarcane industries obtained after the extraction of juice for production of sugar. About 54 million dry tones of bagasse are produced annually throughout the world[7]. It is presently used as fuel for boilers or supplied as raw material for the manufacturing of pulp, paper and building boards. Sugarcane bagasse in its natural state is a poor adsorbent of organic compound such as sugar colorants and metal ion[8]. Bagasse must be modified physically and chemically to enhance its adsorptive properties towards organic molecules or metal ions, routinely found in aqueous solution. This is effectively accomplished by converting bagasse to an activated carbon. In recent years, research interest has increased in terms of the production of low-cost alternatives to activated carbon, which remains an expensive material despite its pro-life use[9-13]. The present work also introduces low-cost alternatives to activated carbon. The efficiency of any adsorbent material to adsorb the targeted compounds (color, ash, colloids) depends on several factors[14-15] such as porosity, surface area, pore size distribution, bulk density, surface chemistry, hardness, pH, particle density, particle size, amount of water soluble minerals and its total ash content. Each of these characteristics may be of special importance depending on the desired use.

The present work is focused on production of activated bagasse fly ash (ABFA) from sugarcane bagasse fly ash by activating with H_2O_2. Since the commercial application of activated carbon is effected by their physical and chemical properties a comparison of the physical and chemical properties of ABFA to those of the commercial activated carbons were carried out.

MATERIALS AND METHODS

The activated charcoal, Darco (reference carbon), was purchased from Sigma, and ion-exchange resin (Indion 830-S) was a gift from Ion Exchange India Ltd. (Mumbai, India). Sugar samples were purchased from Domino, Pvt. Ltd, USA. H_2O_2 (AR) is purchased from Sigma Chemicals. NaCl (AR) and NaOH (AR) are purchased from SD-fine Chemicals.

PREPARATION OF ACTIVATED BAGASSE FLY ASH (ABFA)

The BFA, which is collected from local sugar mill, is washed several times with distilled water to remove the surface adhered particles, dried at 80-100^{0}C. Then different mesh size powders (30, 60, 100, and 200) were separated. The powdered materials were treated with H_2O_2 (100 volume) and allowed to stand for 24 h. at 60^{0}C. The BFA is then washed distilled water for several times and dried at 90-100^{0}C. All the prepared powder was stored in vacuum desiccators for further experiment.

RESULTS AND DISCUSSION

CHARACTERIZATION OF ADSORBENTS

Fourier Transform Infrared (FT-IR) Spectroscopy of ABFA

The FT-IR spectra of the ABFA were scanned in between 500-4400 cm^{-1} and are shown in Figures 1. Some of the bands originating from the sample are characteristics of –OH stretching (3404 cm^{-1}), -CH_2 and - CH_3 asymmetric and symmetric stretching vibrations and carbonyls (1800-1600 cm^{-1}). 1100–1000 and 790–805 cm^{-1} of IR vibration modes are assigned to the major Si-containing functional groups, such as Si-O, Si-C and Si-OH.

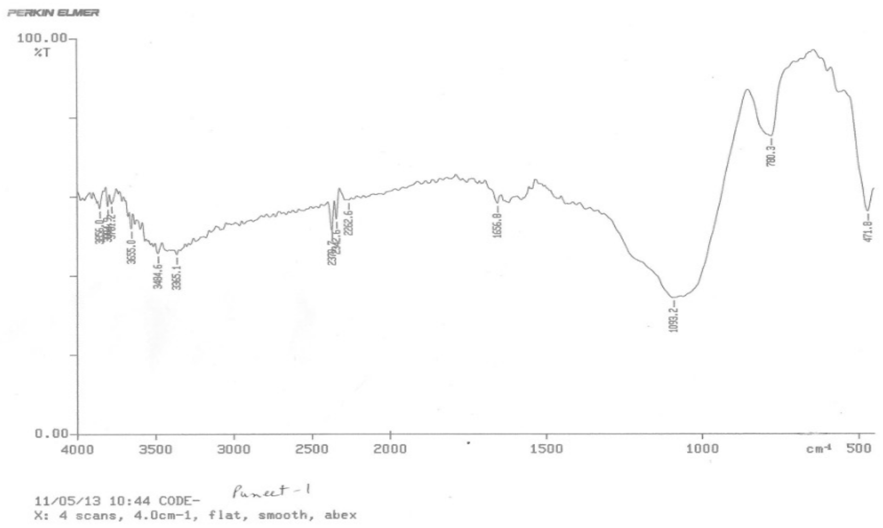

Fig. 1: FT-IR spectrum of ABFA.

Scanning Electron Microscopy (SEM) of ABFA

The SEM images of ABFA shown in Figure 4 clearly demonstrate the porosity and surface texture of adsorbent materials produced from the ABFA. According to Dąbrowski14 a typical definition of pore diameter ranges in different domains are as micropores (<20A); mesopores (20-500A); macropores (>500A).

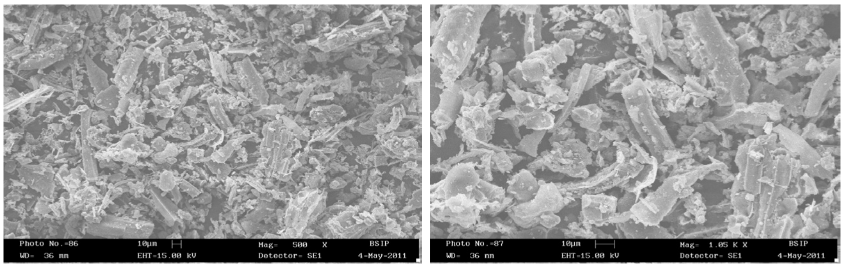

Fig. 2: SEM pictures of activated bagasse fly ash (ABFA) at 100X and 1050X.

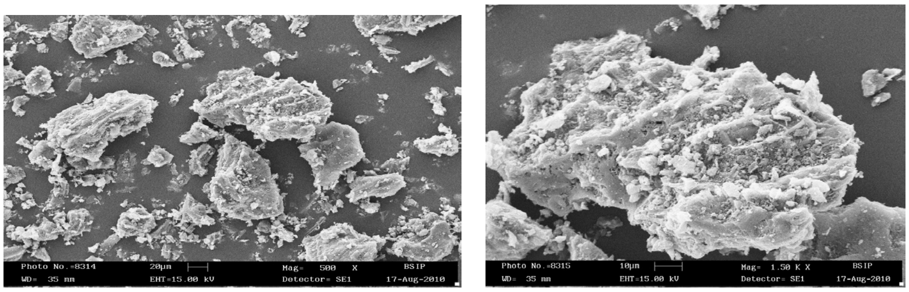

Fig. 3: SEM images of activated charcoal (60-100 mesh size) at different magnifications.

SEM Characterization of Indion - 830 S

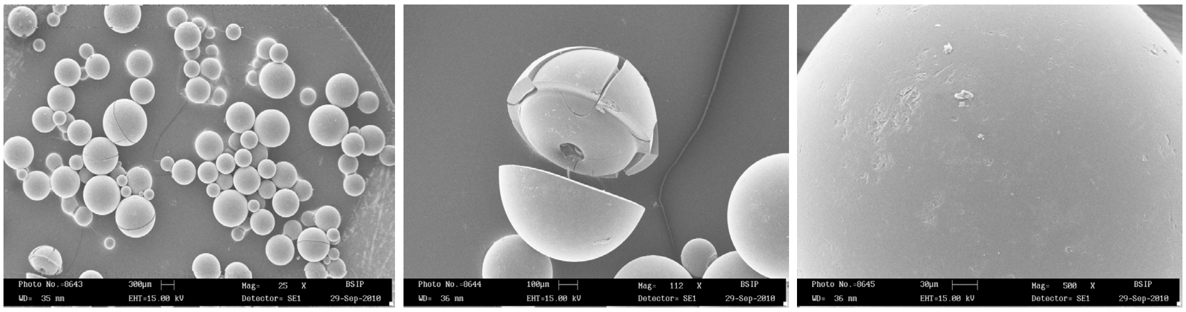

Fig. 4: SEM pictures of Indion - 830 S at 25X, 500 X and 1050 X.

PHYSICO-CHEMICAL AND ADSORPTION CHARACTERISTICS OF ABFA

The physico-chemical properties of ABFA are tabulated in Table 2.

Table. 1: Physical and Chemical Properties of ABFA

Bulk Density (g/ml)	Hardness	Conductivity (μS)	pH	Ash content
0.591 ± 0.005	77.25 ± 0.5	291.60 ± 50	8.14 ± 0.05	6.99 ± 0.05

IODINE TEST

The Iodine Number (IN) (Hassler, 1963) is a relative indicator of porosity in activated carbons. For high surface area carbons (greater than 900 m^2/g), iodine number is numerically similar to BET surface area measurements, whereas for low surface area active carbons, this one-to-one correlation of surface area with IN falls away. The results Table 3 consistent with this statement are observed in the present case. The IN for chars, activated and reference carbons were measured according to the standard test method for activated carbons found in ASTM D 4607-86.

Table 2: PIR of ABFA *Versus* Activated Charcoal

S. No	Amount of Adsorbent (g)	PIR	
		ABFA	Activated Charcoal
1	0.1	15	42
2	0.2	19	60
3	0.3	27	85
4	0.4	29	94
5	0.5	30	97

Molasses Test

The molasses test (Hassler, 1963) results are shown in the following Table 4. A solution of final molasses was treated with the ABFA and the reference carbon of known molasses number. The filtrate absorbance values were measured and molasses number of the sample was evaluated from the ratio of the absorbance values of the sample and the reference carbon.

Table 3: PMCR of ABFA *Versus* Activated Charcoal

S. No	Amount of Adsorbent (g)	PMCR	
		ABFA	Activated Charcoal
1	0.1	3.0	50
2	0.2	5.5	77.32
3	0.3	7.3	89.83
4	0.4	9.6	94.64

Point of Zero Charge (PZC) for ABFA

The amphoteric character of the carbon surface, i.e., to the acidic and/or basic functional groups, the surface potential may be influenced (Radovic et al., 2001) by the pH value of the coexisting liquid bulk phase. The pH value, at which the surface charge is zero, is called the point of zero charge (PZC). For typical amphoteric carbons, the surface is positively charged at pH < pH_{PZC} and negatively charged at pH > pH_{PZC}. Since, pH_{PZC} of ABFA was determined and found to be about 8.5, at any pH < pH_{ZPC}, the surface of ABFA is positively charged and at pH > pH_{ZPC}, the surface is negative.

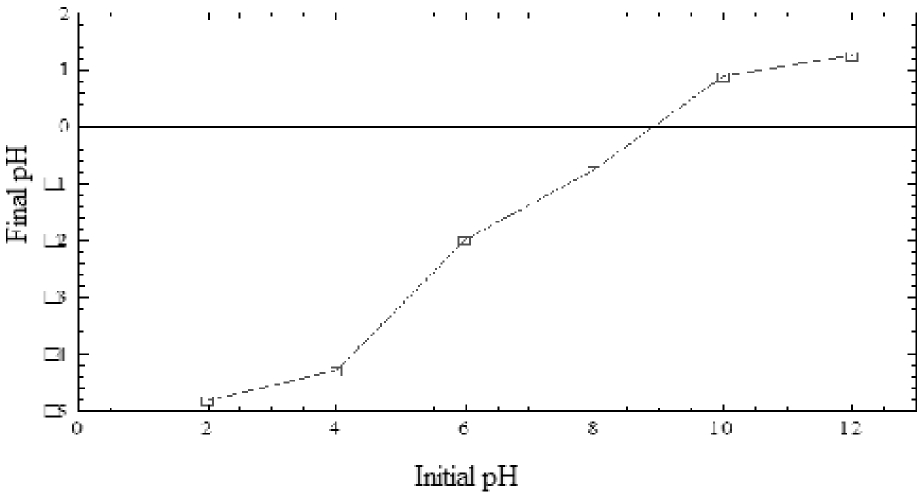

Fig. 8: Determination of the points of zero charge of ABFA using the pH drift method.

ELEMENTAL CHARACTERIZATION

The elemental analysis of ABFA shows the different elemental composition as given in Table 5.

Table 5: Elemental Analysis of ABFA

Element	**% Composition**	
	Present work	**Literature Data (Devnarain *et al*, 2002)**
Carbon		22.36
Hydrogen		-
Nitrogen		30.69
Ash	6.99	-

The chemical composition (Gupta and Ali, 2000) of ABFA was SiO_2 – 60.5%, Al_2O_3 – 15.4%, CaO – 2.9%, Fe_2O_3 – 4.9% MgO – 0.18%. **Batch Mode Adsorption Results**

EFFECT OF CONTACT TIME

The study concerned with relevance of contact time was performed using time interval 2, 4 and 6 hrs. The data included in Table 6-7 illustrate the colour removal efficiency with respect to contact time.

Table 6: Data Showing Decolorization Results of Brown Sugar Sugar (5 ^{0}Brix, pH = 7.0, temp. = 75-80^0 C, shacking = 420 rpm)

Particulars	**Blank**	**ABFA (2g)**		
		Shaking time (hr)		
		2	4	6
Abs at 420 nm	1.804	1.154	0.610	0.449
Color (IU)	36080	23080	12200	8980
Color removal (%)		36	66	75

Table 7: Data Showing Decolorization Results of Brown Sugar Sugar (30^{0}Brix, pH = 7.0, temp. = 75-80^0 C, Shacking = 420 rpm)

Particulars	**Blank**	**ABFA (2g)**		
		Shaking time (hr)		
		2	4	6
Abs at 420 nm	1.505	1.161	0.937	0.730
Color (IU)	5016	38702	3123	2433
Color removal (%)		23	48	51

EFFECT OF PARTICLE SIZE

The study concerned with relevance of particle size was performed using 60, 100 and 200 mesh sizes. The data included in Table 8 illustrate the colour removal efficiency with respect to particle size. The maximum colour removal was found with 100 mesh size ABFA. High rate of adsorption with smaller particle size is due to availability of more specific area on the adsorbent as the process is dependent on the surface morphology (Venkata et al, 2002b). The fine particle size, the larger surface area, which would in turn provide better contact between the adsorbate and adsorbent. Hence, the adsorption capacity would be better.

Table 8: Data Showing the Effect of Particle Size on Decolorization Efficiency (30 ^{0}Brix, ABFA = 2g, pH = 7.0, shacking time = 6 h (420 rpm) and temp. = 75-80^0 C)

Particulars	**Blank**	**Particle Size of ABFA (mesh size)**		
		60	100	200
Abs at 420 nm	1.510	0.946	0.702	1.076
Color (IU)	5033	3153	2440	3585
Color removal (%)		37	52	28

EFFECT OF DOSE

Table-9 shows the effect of adsorbent dosage on the removal of sugar colourants. The percentage of colour removal increased with the increase in adsorbent dosage. This can be attributed to increased adsorbent surface area and availability of more adsorption sites resulting from the increase adsorbent dosage.

Table 9: Data Showing the Effect of Dose on Decolorization Efficiency (30 ^{0}Brix (5090 IU), pH = 7.0, temp. = 75-80^0 C, shacking time = 6 h (420 rpm), mesh size = 100)

Dosage of ABFA (g)	1	2	3	4	5
Color removal (%)	25	51	69	97	98

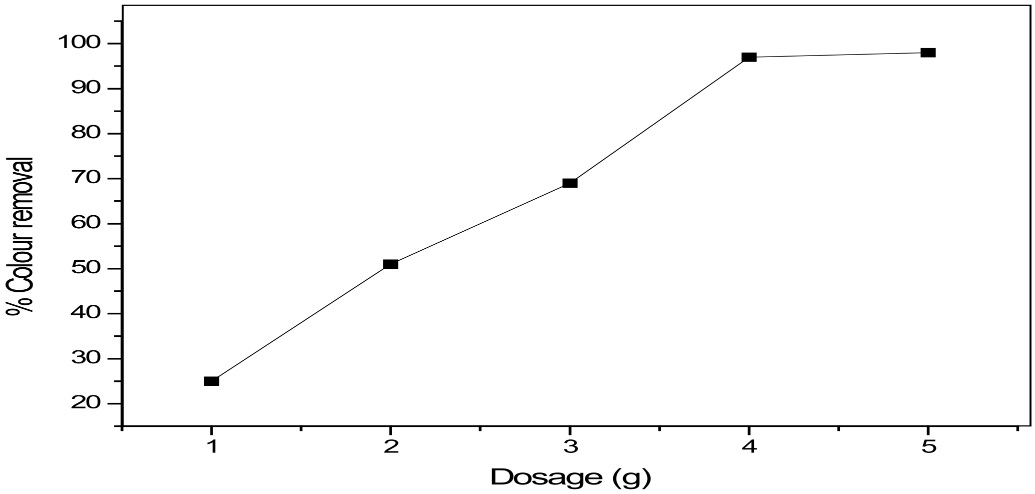

Fig. 9: Effect of dosage on decolorization efficiency of ABFA (30 ^{0}Brix, pH = 7.0, temp. = 75-80^0 C, shacking time = 6 h (420 rpm), mesh size = 100.

EFFECT OF PH

The pH of adsorption medium is one of the most important parameters affecting the adsorption process. Table - 10 shows the effect of pH on the adsorption of colourants (phenolic acid). It was observed that the uptake of colourants by ABFA was almost constant in the pH range of 4.5-6.5. Similar results were reported by Kao *et al.* (2000) and Srivastava *et al.* (2006) for the removal of phenols from aqueous solution by bagasse fly ash and activated carbon. The adsorption decreased with increasing pH. The pH primarily affects the degree of ionization of colourants (phenolics and amino acids) and the surface properties of ABFA. The decrease in colourants (phenolics) adsorption at very low pH (Liu and Pinto, 1997) is due to the increased H^+ adsorption on the carbonyl sites, which suppresses colourants (phenol) adsorption on these sites. At low pH values, the surface of ABFA would be protonated and resulted in a stronger attraction for negatively charge colourants ions (phenolate ions and zwitterons). At high pH, OH^- ions would compete with the colourants molecules for sorption sites. Sorption of excess of OH^- ions could convert an initial positively charged surface of ABFA into a negatively charged surface resulting repulsion of negatively charged colourant ions and consequently adsorption decreased. Similar behavior has been reported in literature (Uddin *at el.,* 2007, Liu and Pinto, 1997) for the adsorption of phenols on the various activated carbons. This could also be due to the increased solubility of phenol molecules at alkaline conditions, which results in greater affinity for the phenol molecules to remain in solution rather than to get adsorbed onto the carbon surface (Vasu, 2008). Unionized colourant molecules would also be attracted, possibly, by physical force (H-bonding).

The effect of pH can also be explained using pH_{ZPC} of the adsorbent. In the present study the p_{HZPC} of ABFA is about 8.5. At any pH < pH_{ZPC}, the surface of adsorbent is positively charged and at pH > pH_{ZPC}, the surface is negative. When the solution pH lowered p_{HZPC}, the phenolate ions are more easily attracted by the positively charged surface of adsorbent, favouring accumulation of phenolate ions on the surface and thus promoting adsorption. On the other hand, when the solution pH exceeded p_{HZPC}, the phenolate ions are repeled by the negative charged surface of adsorbent, hence, adsorption of phenolate ions on the surface is decreased. Similar trends have been reported in literature (Arivoli at el, 2009 and Radovic et al., 2001) in the case of the adsorption of phenols on the various activated carbons.

Table 10: Data Showing the Effect pH on Decolorization Efficiency
(30 ⁰Brix (5033 IU), ABFA = 2g, temp. = 75-80⁰ C, shacking time = 6 h (420 rpm), mesh size = 100)

pH	2.5	4.5	6.5	8.5	10.5
Removal of color (%)	23	43	53	20	13

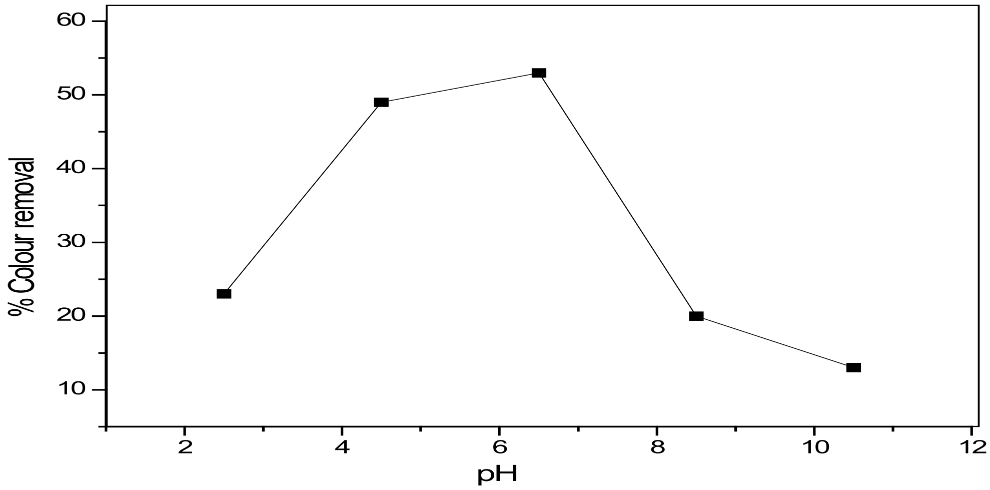

Fig. 10: Effect pH on decolorization efficiency of ABFA (30 ⁰Brix, ABFA = 2g, temp. = 75-80⁰ C, shacking time = 6 h (420 rpm), mesh size = 100).

EFFECT OF TEMPERATURE

The adsorption experiments were performed at different temperatures viz., 30, 40, 50, 60, 70, 80, and 90° C in water-bath shaker (Model-YSI-413-EX). The constancy of the temperature was maintained with an accuracy of ± 0.5° C. The removal of colourants on ABFA increased with increase in temperature (Table 11), suggesting that these processes are endothermic. The maximum removal is occurred in the range of 75 - 85° C.

Table 11: Data Showing the Effect of Temperature on Decolorization Efficiency (30 ^{0}Brix, ABFA = 2g, shacking time = 6 h (420 rpm), mesh size = 100)

Temperature (^{0}C)	30	40	50	60	70	80	90
Removal of color (%)	31	34	36	44	48	53	39

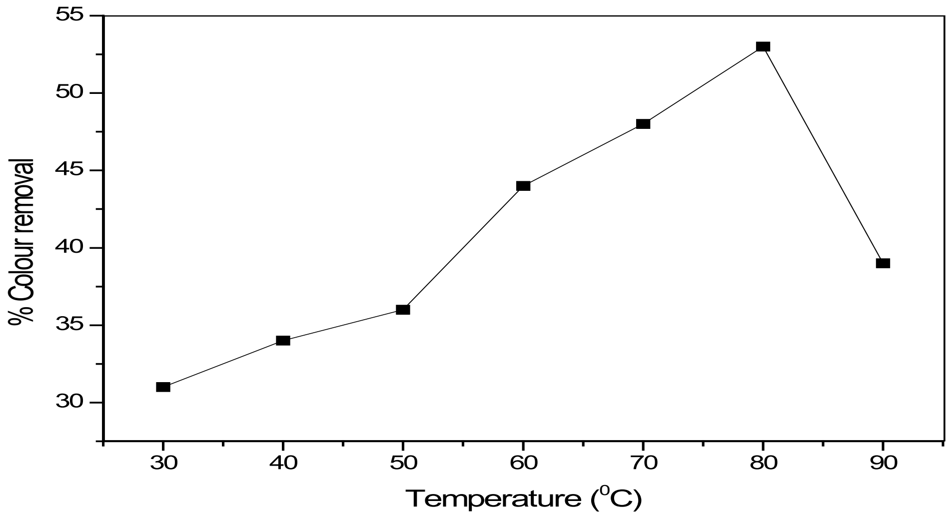

Fig. 11: Effect of temperature on decolorization efficiency of ABFA (30 ^{0}Brix, ABFA = 2g, shacking time = 6 h (420 rpm), mesh size = 100)

EFFECT OF ADSORBATE CONCENTRATION

The adsorption data for the uptake of colourants at different initial concentrations (5, 15, 30, 60 ^{0}brix) is presented in Table 12. The equilibrium data collected in Table 12 reveals that percent adsorption decreased with increase in initial sugar concentration, but the actual amount of colourants adsorbed per unit mass of ABFA increased with increase in sugar concentration. It means that the adsorption is highly dependent on initial concentration of sugar solution. It is because of that at lower concentration, the ratio of the initial number of colurants to the available surface area is low subsequently the fractional adsorption becomes independent of initial concentration. However, at high concentration the available sites of adsorption becomes fewer and hence the percentage removal of colourants is dependent upon initial concentration.

Table 12: Data Showing the Effect of adsorbate concentration on Decolorization Efficiency (pH = 7.0, ABFA = 2g, temp. = 75-80^0 C, shacking time = 6 h (420 rpm) and mesh size = 100)

Brix (Brown Sugar)	5	15	30	60
Removal of color (%)	72	60	51	40

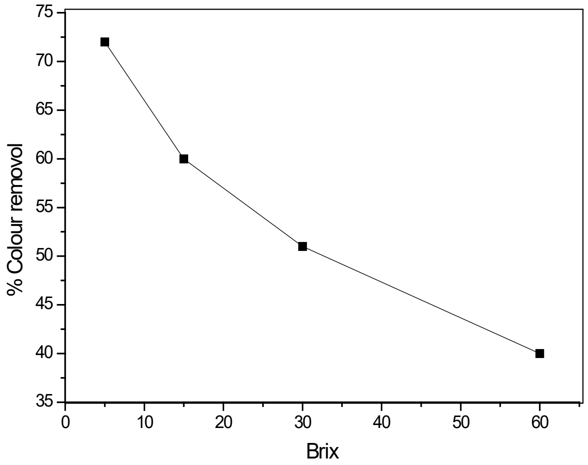

Fig. 12: Effect of adsorbate concentration on decolorization efficiency of ABFA (pH = 7.0, ABFA = 2g, temp. = 75-80^0 C, shacking time = 6 h (420 rpm) and mesh size = 100)

RESULTS OF SINGLE COLUMN EXPERIMENTS

The results of this study are shown in Table 14.

Table 14: Data Showing Colour and Turbidity (30 ^{0}Brix (5045 IU), pH = 7.0, ABFA = 2g, temp. = 75-80^0 C, shacking time = 6 h (420 rpm)

Support	% Colour Removal	Turbidity (NTU)*
Activated carbon	100	4897
Accurel with surfactant	81	467
Ion-exchange resin (Indion 830-S)	80	4526
AMC	50	3142

COMPARATIVE STUDY WITH STANDARD METHODS

In order to compare the performance of ABFA with respect to other standard decolourizing adsorbents, adsorption studies were performed using raw sugar and brown sugar as an adsorbate solutions. Activated charcoal and Indion 830-S were chosen as reference for comparison with the ABFA. The success of any new sugar decolorization process will be based on its colour removal capacity; however, colour removal alone can be misleading as it does not take into account the feed colour. In order to assess the performance of the colour removal capacity of process technology should be used in conjunction with colour loading. Data shown in Table 15 clearly illustrate that load colour index in the case of present process is very high (5055 IU) as compared to the standard procedures, none the less; the adsorption capacity was found to be comparable with conventional adsorbent materials.

Table 15: Comprasion of Processes

Particulars	Adsorbents			
	Accurel	AC	Resin	ABFA
Feed colour (IU)	1500	1000	3000	5055
Colour removal %	85	90	78	52

COST ANALYSIS

Since sugarcane is produced all over the world. So, the raw material is available in abundance. Comparison of the new adsorbent was done with a standard commercial carbon (activated charcoal). For synthesis of 1 kg of ABFA from BFA costs approximately Rs. 230/- whereas activated charcoal costing approximately Rs.1836/-. Hence, new kind of adsorbent is relatively cheaper than the commercial adsorbent.

CONCLUSION

Bagasse fly ash, a waste material generated in the sugar industry, is a low cost and effective adsorbing surface for the removal of sugar colourants. The proposed process is, in one broad embodiment, a process for the removal of impurities from an aqueous sugar solution comprising contacting the solution with the new adsorbent derived from a cheap, and abundantly available renewable source (bagasse). The removal of colourants from aqueous sugar solution using ABFA takes place by a particle deffusion mechanism. The described method could form the basis of a practical industrial- scale process for new kind of decolorizing agent for its application in sugar refining.

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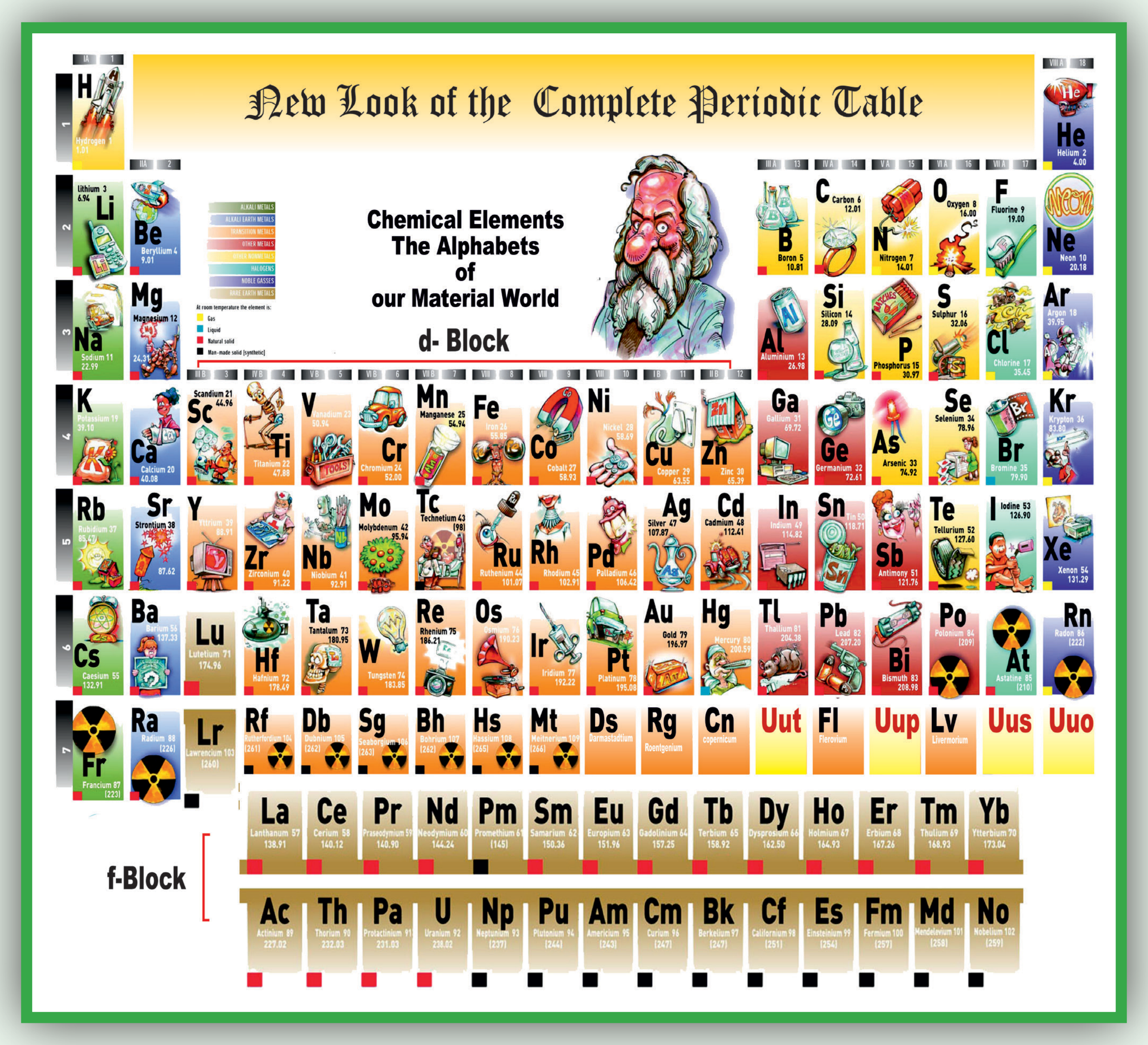
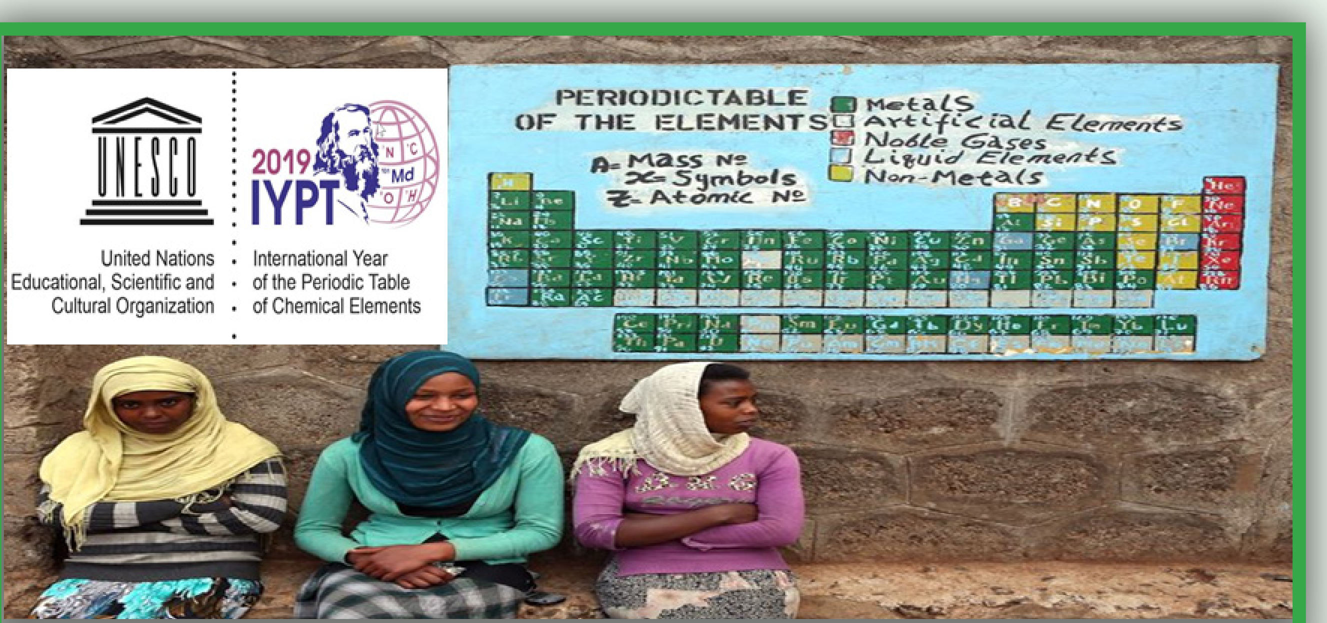
THE COMPLETE FORM OF THE PERIODIC TABLE



INTERNATIONAL YEAR OF PERIODIC TABLE (IYPT)



1869 is considered as the year of discovery of the Periodic System by Dmitri Mendeleev. 2019 has been declare the 150th anniversary of the Periodic Table of Chemical Elements and has therefore been proclaimed the "International Year of the Periodic Table of Chemical Elements (IYPT2019)" by the United Nations General Assembly and UNESCO.

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