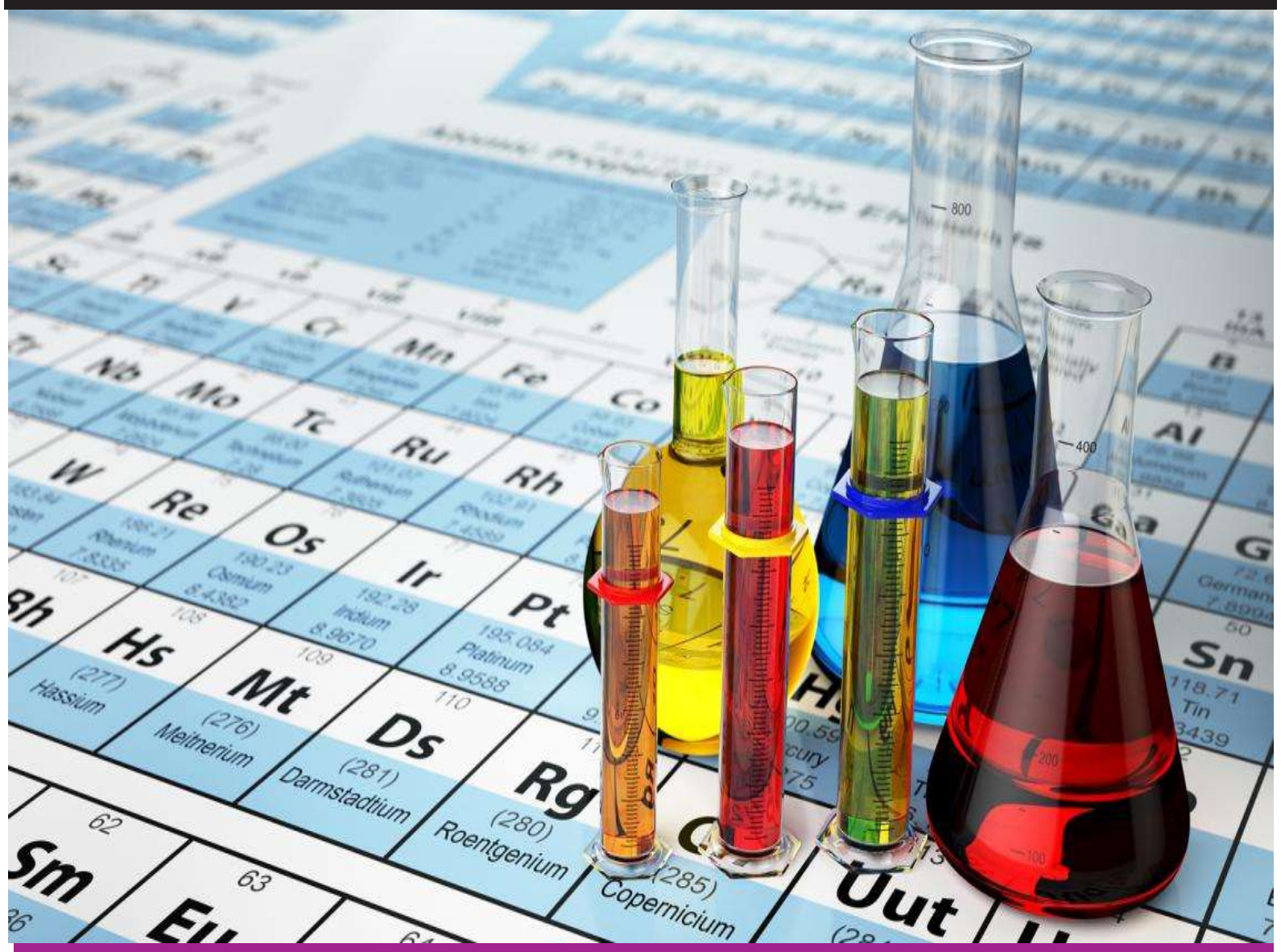
ASSOCIATION OF CHEMISTRY TEACHERS

NEWSLETTER

ISSUE : 19 JANUARY - APRIL 2021



Promoting Excellence in Chemistry Education

Association of Chemistry Teachers

News Letter, January - April 2021

Contents of the News Letter : Issue -19

From Editorial Desk

Prof. Wasudeo Gurnule
Editor
Kamla Nehru Mahavidyalaya,
Nagpur, Maharashtra.

We are happy to inform that the contributions of ACT ranges from International Olympiads, organizing seminars, science exhibitions, workshops, expert invited talks, innovating conceptual science experiments, conferences, talent search examinations, training faculty and students etc. We are bringing in the present issue of the newsletter with the reports on the ACT activities, trends in chemistry, views and news. We have included three scientific articles in the present issue. We have also included reports on National Chemistry Events. Reports on National Science Day Celebrations were also given briefly.

We invite good suggestions and better contributions from the readers to get best output of the future issues. We welcome you all to participate in the second research convention.

Members of Editorial Board

Honorary Members of ACT

We have great pleasure in bringing the updated list of honorary members of Association of Chemistry Teachers, who are sources of inspiration, guidance and support in activities of ACT.

The editorial board of ACT News Letter is proud of the academic achievements of these legendary honorary members.

Bharat Ratna Prof. C.N.R. Rao, FRS
National Research Professor : Linus Pauling Research Professor,
Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bengaluru - 560 064
E-mail : cnrrao@jncasr.ac.in

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E-mail : profmmsharma@gmail.com

Padma Vibhushan Dr. R.A. Mashelkar, FRS
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President, Global Research Alliance, National Chemical Laboratory, Pune - 411 008.

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Padma Shri Prof. Jai P. Mittal
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Chairman, Academic Board, UM-DAE Centre for Excellence in Basic Sciences,
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Prof. Mihir K. Chaudhuri
Former Vice-Chancellor, Tezpur University, Tezpur.
Advisor, Education Department of Government of Assam, Gawahati - 781 006
E-mail : chaudhurimihirk@gmail.com; mkc@tezu.ernet.in

ACTIVTIES OF ACT

Workshop on Awareness and Measures of Fluoride in Drinking Water

A one day workshop on 'Awareness and Measures of Fluoride in Drinking Water' was organized at **Telangana Social Welfare Residential College for Women,** Suryapet on **February 8, 2021.**

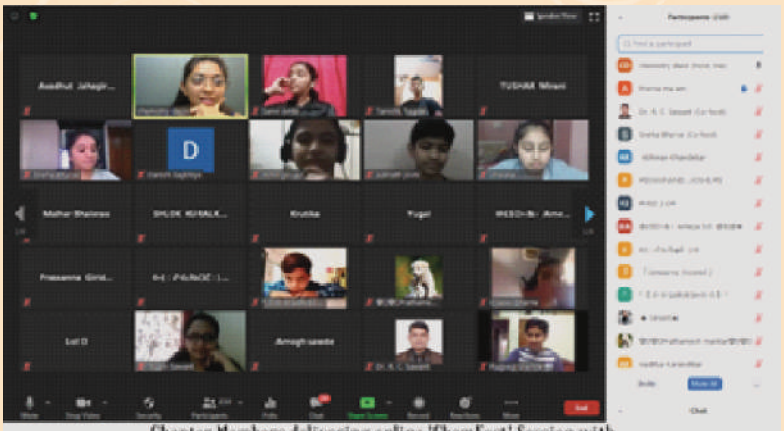
Dr. Mannam Krishna Murthy, Chief Executive Dean, Varsity Education Management Ltd., Hyderabad and Secretary ACT South Zone Coordinated all academic events related to the workshop. The theme of the workshop was based on the local water pollution problem. Students were allowed to participate physically by maintaining COVID precautions.

ChemInspire 2020

In order to develop curiosity and scientific spirit about chemistry among school children , ACS International Student Chapter, Dr Ambedkar College, Nagpurin collaboration with Association of Chemistry Teachers (western zone) organised ACS Chemistry Festival ChemInspire 2020 . The program was conducted from December 2020 to March 2021. M Sc and B Sc student chapter members worked on various interesting chemistry experiments..

Overall, “ChemInspire 2020” received a participation of around 1850 participants making it a grand success by meeting the objectives and goals. ACS chapter students were guided and

supervised by Dr Hemant Pande, Vice President, Association of chemistry teachers , Former Head, Dept. of Chemistry, Hislop College and Advisor of the program, Dr Deepa Panhekar, HOD Chemistry and Head, ACS Intl. Student Chapter, DACN, Asst. Prof Dr R C Sawant and Mr Parag Panse.



Chapter Members delivering online 'ChemFest' Session with
B R Mundle School
With the participation of around 210 Students

Role of Chemistry in Day-to-day Human Life

A one day seminar was organized jointly by Rashtriya Madhyamik Shikshan Abhiyan, Telangana and Association of Chemistry Teachers, Mumbai on the 'Role of Chemistry in Day-to-day Human Life' at Telangana Model School, Junior College, Bothalapalem village, Nalgonda Dist., on 9th February 2021.

Dr. Mannam Krishna Murthy, Secretary ACT South Zone from Varsity Education Management Ltd., Hyderabad acted as convener of the seminar, who also gave the key-note address and presented a brief account of ACT academics.

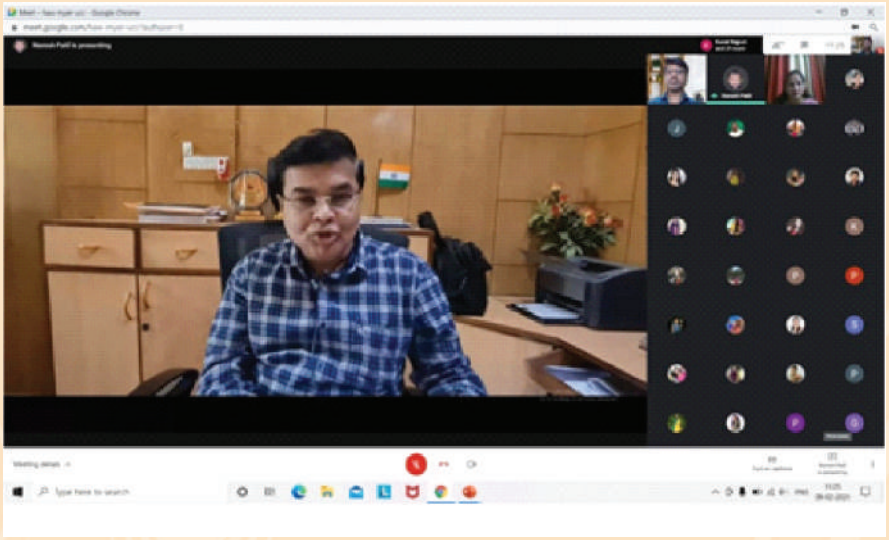
Mr. P. Azaraiah, Principal TMSJ College, Damaracherla acted as Chair person and inaugurated the seminar. Dr. V. Venkateswarlu, HOD Chemistry, KNM Government Degree College, Miryalaguda graced the occasion as chief guest and briefed on the knowledge of various branches of Chemistry.

Report on International Webinar on Empowering Diversity in Science GWB-2021

ACT ORGANIZES GLOBAL WOMEN'S BREAKFAST - 2021

International Webinar on Empowering Diversity in Science
organized by
Department of Chemistry, Kamla Nehru Mahavidyalaya, Nagpur
and Association of Chemistry Teachers (ACT)

Webinar organized by
Department of Chemistry of Gokhale Education Society's
RNC Arts, JDB Commerce and NSC Science College, Nashik Road, Nashik
In collaboration with
Association of Chemistry Teachers (ACT),
C/o. HomiBhabha Centre for Science Education (TIFR), Mumbai
2021 IUPAC Global Women's Breakfast Empowering Diversity in Science
on
Tuesday 9 Feb 2021, At 11.00 am on Google Meet platform



IUPAC Global Women Breakfast GWB-2021
Sant Gadge Baba Amravati University, Amravati

IUPAC GLOBAL WOMEN'S BREAKFAST: GWB 2021

Theme : "Empowering Diversity in Science"

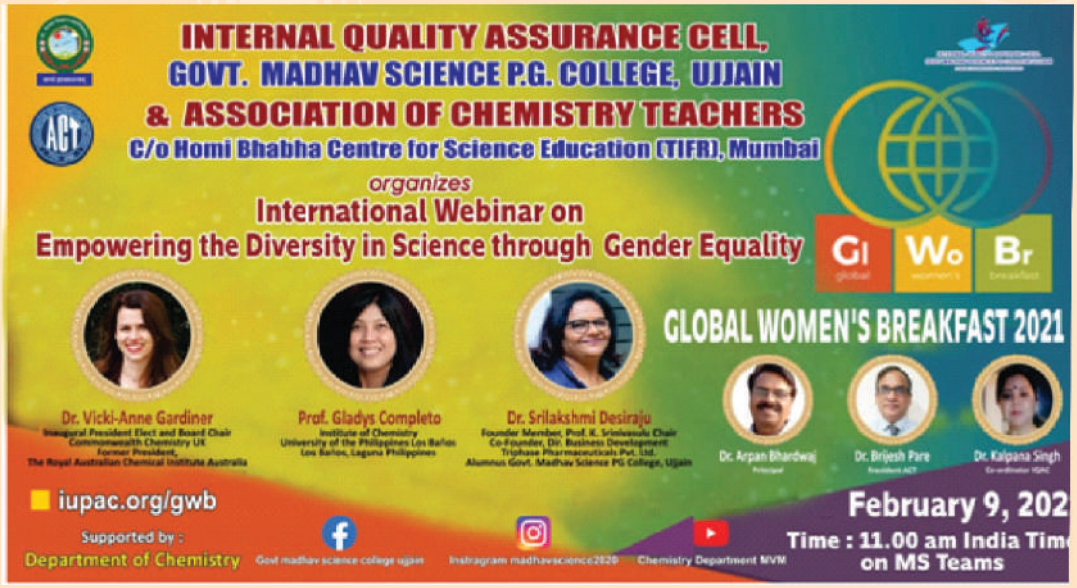
Webinar on Contribution of Women in Chemical Sciences

Promoted by

Association of Chemistry Teachers

c/o HomiBhabha Centre for Science Education (TIFR), Mumbai Organized by Department of Chemistry Sant Gadge Baba Amravati University, Amravati

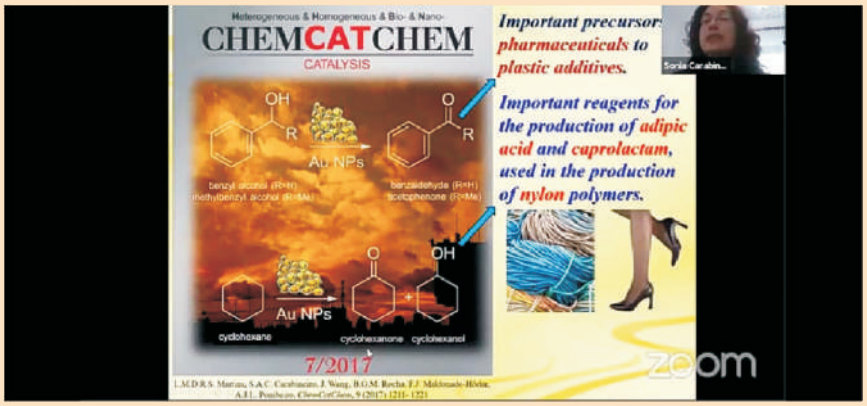
International Webinar on
Empowering the Diversity in Science Through Gender Equality
Organized by
IQAC, Govt. Madhav Science PG College, Ujjain
and
Association of Chemistry Teachers

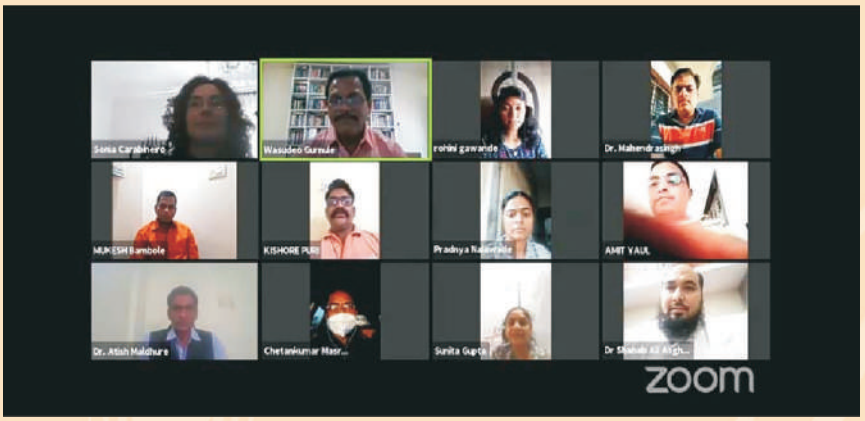


NATIONAL AND INTERNATIONAL ACTIVITIES OF ACT
Webinar organized by
Department of Chemistry
Christ Church College, Kanpur
in Association with IUPAC and ACT

International Webinar on Sustainable Chemistry
organized by
Association of Chemistry (ACT) Mumbai

International Webinar
on
Innovations in Science and Technology
organized by
Department of Chemistry,
Smt. Narsamma Arts, Commerce and Science College, Amravati
and
Association of Chemistry Teachers (ACT) Mumbai





AWARDS

Prof. R. S. Mali Awarded Life Time Achievement Award

Honorary Member of ACT Prof. R. S. Mali, Pune received Lifetime Achievement Award from Savitribai Phule Pune University on 10th February 2021 on occasion of 72nd Foundation Day of the University for achievement in Higher Education and Administration.

Dr. Kothari Wins National ICT Award

Government teacher Dr. Yogendra Kumar Kothari has been selected for the prestigious National information and communication technology (ICT) award. National ICT award aims to motivate school teachers. This ICT awards for teachers for using ICT for innovations in Education are presented by Ministry of Education, Government of India, Central Institute of Educational Technology , National Council of Educational Research and Technology, New Delhi.

The award proposes to recognized teachers who have promoted learning among students by effectively and innovatively integrating technology-enabled teaching into school curriculum and subject teaching. As per the guidelines of the Ministry of Education a jury was constituted at National level to select the teachers for the National ICT awards for the year 2018 and 2019. The jury evaluated 205 entries received from 28 states/ Union Territories and 5 autonomous bodies during 5 to 11th February 2021 for presentation in online mode, out of which 10 teachers were from Madhya Pradesh. After thorough consideration and evaluation on the basis of detailed online presentation made by teachers about their work as well as their interaction in ICT, the Jury selected 49 teachers, out of which Government Madhav Nagar School of Excellent Lecturer Dr. Yogendra Kumar Kothari was selected for the National ICT Award.

Academic participation of ACT Members

1. Prof. Brijesh Pare, President of ACT, delivered a talk on Can one LEARN to be Innovative?, in International Webinar organized by Department of Chemistry, Smt. Narsamma Arts, Commerce and Science College, Amravati on 27th February 2021
2. Dr. Amar Shrivastava, EC Member of ACT, North Zone, delivered a talk in Creating Assessment using PaperShala, in Live interaction Webinar, on 15th March 2021.
3. Prof. M. Swaminathan, EC Member of ACT, South Zone, delivered a talk in Webinar on Fluorometric Analysis and Its Application organized by Department of Chemistry, SRM Institute of Science and Technology, Chennai, on 26th April 2021.
4. Prof Mannam Krishnamurthy, Secretary of ACT, South Zone, delivered a talk on Li-Ion battery electrolyte degradation characterization by mass spectrometry, in Chemistry World Webinar, on 8th June 2021.
5. Prof. Wasudeo Gurnule, Secretary of ACT West Zone, delivered a talk on SBR-Antomony Oxide Rubber Nanocomposite, in International Webinar organized by Department of Chemistry, Smt. Narsamma Arts, Commerce and Science College, Amravati on 27th February 2021.

Trends in Essential Oils in Cosmetic Formulations

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Kamla Nehru Mahavidyalaya,
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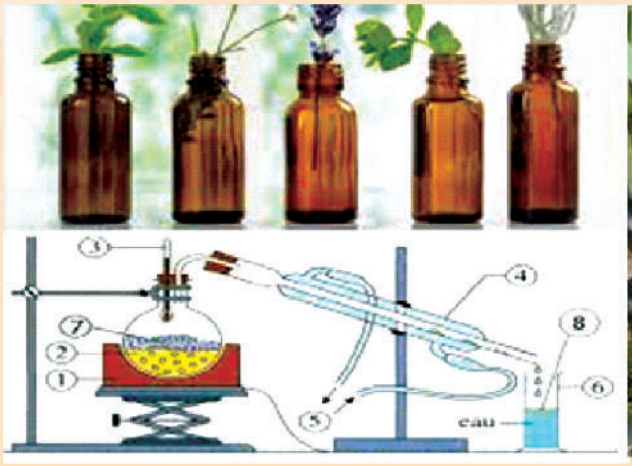
Essential oils are complex chemical mixtures of volatile compounds produced by plants and isolated by physical means (hydro/ steam distillation/ expression/ solvent extraction/ Super Critical Fluid Extraction etc.) from a whole plant or plant part of known taxonomic origin. They are concentrated hydrophobic liquids containing volatile aroma compounds from plants. Essential oils are also known as volatile oils. The oils carry a distinctive scent or essence of the plant.

Essential oils are produced by blossoms, leaves, and fruits of different plants and stored in special tissues such as glandular hairs, oil cells, oil receptacles

(for example, alcohols, aldehydes, ethers, ketones and phenols), homologues of phenylpropanoids, as well as minor amounts of diterpenoids and miscellaneous volatile organic compounds.



The antimicrobial properties of essential oils have been known for many centuries. In recent years, a large number of essential oils and their constituents have been investigated for their antimicrobial properties against some bacteria and fungi. It is reported that essential oils provide a gentle and inexpensive way of treating acne, clearing infections and healing acne scarring. Hence essential oils can prove to be beneficial in antiacne formulations and skin care cosmetics.

For essential oils, antibacterial, antifungal, anti-inflammatory, anti-rheumatic, antitussive, antiviral, expectorant, sedative and blood-circulation-enhancing effects have been described. They are able to improve odour of cosmetic preparations, and they may act on cognition, memory and mood. It is commonly accepted that the biological activity of an essential oil is the result of both its active and inactive substances. Inactive substances may influence resorption, skin penetration, rate of reaction, or bioavailability of the active compounds. In addition, several active compounds may have a synergistic effect. Furthermore, the biological activity of a given essential oil may also be influenced by factors related to the medicinal plant as well as to environmental and agronomic conditions. The means of application of essential oils depends on the pathophysiology, the desired outcome, safety and toxicity data as well as cultural preferences. The utilization of the essential oils of plants is widespread, ranging from perfumes, fragrances, spices, cosmetics and medicinal.

Nowadays, essential oils are the subject of intensive scientific research and also attract attention of cosmetic and pharmaceutical industries due to their potential as active pharmacological compounds or natural preservatives. Enormous diversity of this group of natural compounds and wide spectrum of biological properties make them attractive for many industries and new areas of application still has not been discovered. Regardless from sensory properties of essential oils, antimicrobial and antifungal activities are the goal of research. A new promising field of application of essential oils as natural preservatives in cosmetics or feed additives in human or animal food or as plant protection products has been studied. It is estimated that more than 3000 essential oils are of commercial importance and used in flavour, chemical and cosmetic industries.

Essential oils are often used to ease stress, boost mood, relieve pain from headaches and migraines, get a better night sleep, quell nausea, and even repel insects. The beneficial compounds in the oils are often delivered through three main pathways: inhalation, topical application to the skin, and oral ingestion under expert supervision.

Essential oils are sometimes applied to the skin directly. This can be useful for delivering oils to a specific problem area, such as a backache, wrist pain, or sinus troubles. However, the topical use of essential oils should be done with caution. Formulations including essential oils such as ointments, gels, pastes, various skin and hair care preparations should be formulated by considering the suggested use levels of concerned essential oils as improper concentration may lead to undesirable properties of the formulation.

Essential oils can be irritating to the skin and should not be applied full-strength on the skin. They should be diluted in carrier oil (such as almond, apricot kernel, or avocado oil etc.) before being applied to the skin.

Essential oils are being used in various cosmetic preparations such as soaps, lotions, creams, shampoo, ointments, hair oils, massage oils, bath salts etc. and may be used during massage, spa treatments, some other aromatherapy applications, compress, or spot treatment depending upon their properties, uses and use levels.

Essential oils of Clove, Cinnamon and Ajowan are showing a very good antiacne property and thus finds application in antiacne creams. Cinnamon oil possesses Antidandruff property and can be used as Antidandruff agent in shampoo formulations. Cinnamon oil can be used in cream formulations for improvement in texture of skin and restoring normal skin colour on the face. Clove oil, Cinnamon oil and Ajowan oil have potential to be used as natural preservatives as a substitute for synthetic preservative for preservation of shampoo and cream formulations.

Some common examples of essential oils and their trends in cosmetics includes- Sandalwood oil, which can be used for its healing, antiseptic, anti-inflammatory, calming, soothing and rejuvenating properties in various cosmetic preparations. Rose oil can be used in cosmetic preparations to hydrate dry skin, clear acne, reduce signs of aging, minimize the appearance of scars, and help with conditions such as eczema and rosacea also known as mood elevator and reduces anxiety. Chamomile oil is used to improve mood and gives relaxation, known in cosmetics for its antibacterial, anti-inflammatory, skin lightening and antiaging properties. Ylang-Ylang oil is used in aromatherapy for reducing skin inflammations, irritation and mood enhancer,known in cosmetics for its antiseptic, antiaging and also for skin and hair oil balancing properties. Tea Tree oil can be used to treat skin conditions such as spots, pimples, blemishes, dryness, and infections. Bergamot oil, is known for anti-bacterial, anti-inflammatory, and analgesic properties, can be used

to improve skin conditions like eczema, acne and spots in various topical applications. Lemon oil can be used as antibacterial, antifungal, conditioning, astringent, fragrant, anti-cellulite, complexion enhancer in cosmetic formulations.Carrot Seed oil can be used in cosmetics, this oil is reported to have antibacterial, antifungal, antioxidant, moisturising and anti-inflammatory properties.Cinnamon oil research suggests the oil of this popular spice may be used for treating acne, dandruff, ease stress, relieve pain, fight off infections, and can improve skin tone.Citronella oil is deodorant, insect repellent, can enhance skin complexion, used in anti-lice and anti-acne preparations. It is also mood enhancer, used in perfumery.Clove oilis used to treat skin infections, acne, toothaches, and relieve pain.Eucalyptus oil, the active ingredient in VapoRub, eucalyptus is commonly used to treat colds, congestion, and coughs, and is being studied for antibacterial and stimulant benefits. It can be used for skin rejuvenation and acne treatment.Geranium oil, commonly used in skincare, perfumery and research shows this floral oil has antimicrobial properties.Grapefruit oil, is citrus oil can be used in aromatherapy to reduce stress, stimulate circulation, increase energy, enhance mood. It can also be used to treat acne, reduce fine lines on skin and in anticellulite preparations.Jasmine oil, a sweet-smelling floral oil, it is used as a stress-reliever with potential to help treat skin conditions including aged and dry complexions, inflammation, oily conditions, and psoriasis and commonly used in perfumery.Lavender oil, one of the most widely used essential oils, used as perfume. Lavender oil is known for anti-inflammatory, anti-ageing and moisturising properties. Neem oil is used to treat fungal infections, acne, dandruff and minimizes scars. It is widely used in skincare and hair care products. Neroli oil is known to reduce ageing sings, stretch marks, spots, act as moisturiser, helps in treating acne and associated redness. Orange oil is used in perfumery. Improves acne skin condition, helps in skin exfoliation. It has rejuvenating, antiseptic and anti-inflammatory properties. Peppermint oil has antiseptic, antibacterial properties, also has cooling, soothing and astringent abilities and used as component of fragrance in many cosmetics. Rosemary oil known to stimulate hair growth and soothes inflammation. Basil oilis known for its anti-inflammatory and blood purification property and can be used to treat acne, dandruff and also known as hair growth promoter.

The list goes on, as India has a rich heritage of traditional remedies and if research continues in deep study of essential oils, we can get more promising properties of a greater number of essential oils to be used in variety of formulations. And the products containing essential oils are having great future asin recent years there has been an increasing interest in the use of natural substances, because of their relatively safe status and wide acceptance by consumers.

Artificial Intelligence

Dr. M. R. R. PRASAD
Scientist – SF (Retired),
ISRO and Life Member ACT –
Southern Zone.

What is Artificial Intelligence (AI)?

Artificial Intelligence is an interdisciplinary science with multiple approaches. It is a wide-ranging branch of computer science concerned with building smart machines capable of performing tasks that typically require human intelligence. It is an attempt to replicate or simulate human intelligence in machines. Advancements in machine learning and deep learning are creating a paradigm shift in virtually every sector of the industry.

Norvig and Russell classified the four different approaches that have historically defined the field of AI:

1. Thinking humanly
2. Thinking rationally
3. Acting humanly
4. Acting rationally

The first two ideas are concerned with the thought processes and reasoning, while the others deal with behavior.

Patrick Winston, the Ford professor of artificial intelligence (AI) and computer science at MIT, defines AI as "algorithms enabled by constraints, exposed by representations that support models targeted at loops that tie thinking, perception and action together." Research in AI has focused mainly on the following components of intelligence: learning, reasoning, problem solving, perception, and using language.

Methods and Goals in AI:

Symbolic vs. connectionist approaches

AI research follows two distinct, and to some extent competing methods. The symbolic or otherwise known as the “top-down” approach; and the connectionist or alternately known as the “bottom-up” approach. The top-down approach seeks to replicate intelligence by analyzing cognition independent of the biological structure of the brain, in terms of the processing of symbols—therefore the symbolic label. The bottom-up approach, on the other hand, involves creating artificial neural networks in imitation of the brain's structure—and hence the connectionist label. In simple terms, neural activities are the basis of the bottom-up approach, while symbolic descriptions are the basis of the top-down approach.

Strong AI, Applied AI, and Cognitive Simulation:

Strong AI aims to build machines that think. The ultimate ambition of strong Artificial intelligence is to produce a machine whose overall intellectual ability is indistinguishable from that of a human being.

Applied AI, also known as advanced information processing, aims to produce

commercially viable “smart” systems. Applied AI has enjoyed considerable success. There are many commercial smart systems, including programs for medical diagnosis, financial management, credit authorization, corporate planning, financial document routing, computer installation design, automobile design and manufacture, camera lens design, airline scheduling, cargo placement, oil and mineral prospecting, chemical analysis, and genetic engineering, automatic help services for home computer owners.

In cognitive simulation, computers are used to test theories about how the human mind works -for example, theories about how people recognize faces or recall memories. Cognitive simulation is already a powerful tool in both neuroscience and cognitive psychology.

Note : It is a summary of on-line literature for the benefit of readers.

Fluorimetric Technique – A Highly Sensitive Analytical Tool to Explore Excited State Characteristics

Prof. M. Swaminathan
Nanomaterials Laborotry,
International Research Centre,
Department of Chemistry,
Kalasalingam Academy of Research and Education,
Krishnankoil-626126

An organic molecule on optical absorption gets electronically excited from the ground state to singlet state. This electronic excitation may lead to the change in the physical and chemical characteristics such as dipole moment, structure, geometry, acidity and reactivity of the organic molecule. How to find out and analyze these characteristics in the excited state? Only technique available for the study of excited state characteristics is fluorescence spectroscopy. This can be understood from the origin of fluorescence spectrum. In this article, importance and utilization of fluorimetric technique on the study of excited state characteristics are outlined with example.

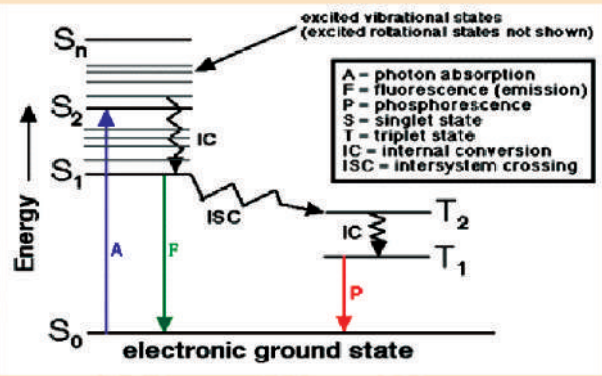


Figure 1 – Jablonski Diagram

Jablonski diagram clearly illustrates origin of absorption spectrum, fluorescence spectrum and phosphorescence spectrum of a molecule. As the absorption of a molecule (represented by blue line) occurs from the ground state So, it reflects the ground state characteristics of a molecule. Hence the ground state properties of a molecule can be analyzed by its adsorption spectrum. After excitation to any of the higher singlet states

(S_1, S_2, S_3 ....) by light, molecule comes immediately to lowest vibrational (V_0) state of S_1 by vibrational relaxation and then loses energy by emission of light. This radioative emission from $S_1(V_0)$ state to any of the vibrational level of ground state (S_0) is called fluorescence (Green line). Since the fluorescence originates always from excited singlet state (S_1), fluorescence spectrum reflects the properties of a molecule in the excited singlet state and it is also independent of excitation wavelength. If a molecule undergoes any change in physical or chemical properties on excitation, its excited state characteristics can be determined and analyzed only by florescence spectrum. By intersystem crossing, the molecule from $S_1(\nu_o)$ State may go to triplet state (T_1) and it may loose energy from $T_1(\nu_0)$ state to any of vibrational states of S_0 by radiative or non - radiative process. The emission from $T_1(\nu_o)$ state to ground state is called phosphorescence (red line). As it is possible to analyse micro molar (10^{-6} M) solutions by fluorescence, it is considered as a highly sensitive technique. **Hence fluorescence is considered to be a highly sensitive and only analytical tool to study the excited state characteristics of a molecule.**

Though both UV-Visible absorption and fluorescence spectroscopy are analytical tools, applications of UV-Visible absorption spectroscopy is limited as it has limited parameters. But in Fluorescence spectroscopy more than fourteen parameters have been identified and they had been used for clinical, biological, environmental and sensor applications. In this article some commonly used parameters such as emission spectrum, excitation spectrum, Stokes shift, life time and, quantum yield and their application in the study of excited state properties are described briefly to realize the importance of fluorimetric technique.

Fluorescence Parameters:

Fluorescence Emission spectra : Emission is scanned by exciting a molecule with a particular wavelength (λ_{ex} - Fixed). In Fluorescence Emission spectra, its Shape, peak position and fluorescence intensity can be used to infer the properties of molecules in the excited state.

The intensity of fluorescence I_f varies with Instrument

$$I_f = I\,A\,\phi \qquad \text{.....(1)}$$

I - Intensity of Excitation light, A - Absorbance at λ_{exi}, ϕ - Quantum yield

Calibration graph is a must for quantitative analysis of a fluorescent compound. Shape and peak position are characteristics of a compound.

Fluorescence Excitation spectra: Excitation is scanned by monitoring emission at a particular wavelength(Wavelength of emission (λ_{em}- fixed). As the emission depends upon the absorbance at excitation wavelength, excitation spectrum should exactly match with the **absorption spectrum**, if there is no change in shape and structure of the molecule during excitation.

Stokes shift - Difference in frequency of absorption and emission maxima (Wave number scale) is called as stokes shift. Stokes shift gives an idea of the extent of relative stabilization of the ground state and the emissive state in the solvent medium.

Fluorescence quantum yield : Fluorescence quantum yield, varying from 0 to 1, is an important parameter and characteristic of fluorescing molecules (Fluorophores).

ϕ_f = fluorescence quantum yield.

Absolute Quantum yield = Fluorescence at all and at all directions/ Light absorbed

As it is very difficult to measure Absolute quantum yield of fluorescence, relative quantum yield is used for practical applications. From absolute quantum yield of some representative fluorophores (1), the relative quantum yield is determined for other fluorophores (2) by applying equation 1 for each fluorophore. Quinine sulphate is taken as standard representative fluorophore for which quantum yield was determined and reported.

I_f of $F_1 = I_1 A_1 \phi_1$, $\phi_1 = \phi_2$ of Quinine sulfate = 0.55 (Quinine sulphate in 0.1 N HCl)

$F_2 = I_2 A_2 \phi_2$

When ex is same for both fluorophores, $I_1 = I_2$

$$F_2 / F_1 = A_2 \phi_2 / A_1 \phi_1; \quad \phi_2 = F_2 A_1 \phi_1 / F_1 A_2$$

F_1 and F_2 are determined from the area of fluorescence curves. Substituting absorbencies at excitation wavelength (A_1 and A_2) , F_1 and F_2 , relative quantum yield of unknown fluorophore (ϕ_2) can be obtained .

Fluorescence Lifetime : Lifetime of excited singlet state I_O is measured easily by single photon counting method using time resolved spectrofluorimeter.

The fluorescence lifetime $\tau_f = \tau_0 \phi_f$, If $\phi_f = 1$; $\tau_f = \tau_0$

Quantum yield and lifetime are used as powerful tools for investigating the dynamical processes of the excited state.

Applications : How these parameters are used for the determination of fluorescent molecules and to study their excited state properties?

Highly sensitive technique - Concentration of a fluorophore can be determined up to 10^{-6} M or even at less concentration depending on its quantum yield. As the intensity of fluorescence is an arbitrary unit and differs for each instrument, a calibration graph of I_fVs [C] is a must for the determination of flurophore concentration. Based on the fluorescence intensity, concentration of the flurophore can be determined from the calibration graph. Two samples having similar absorption spectra may be distinguished if they fluoresce at different wavelengths. Some of the non-fluorescent biological molecules like some proteins can also be identified and analyzed fusing highly fluorescent molecules as fluorescent probes with non-fluorescent proteins. Some commonly used fluorescent probes are Rhodamine B and Fluorescin.

Excited state properties :

Excited state acidity constants : The ground state acidity constant, pKa, is 9.8 for 1-Naphthol , but its excited state pKa* was found to be -1. Acidity of 1-Naphthol increased so much on excitation. A number of organic compounds with acidic and basic groups were analyzed fluorimetrically and found that compounds containing -OH , -SH , $-NH_2$, NH (- ϕ) groups became stronger acids and weaker bases in S_1 state than S_0 state and -COOH, -COR, -CSR, = N- (- ϕ) become stronger bases in S_1 state than in S_0.Two methods are commonly used to determine the excited singlet state pKa (pKa*) values.

1. **Forster cycle method (Theoretical) :** This method uses absorption or fluorescence maxima in wave number for acid (BH, ν_{BH}) and its conjugate base (B^-, ν_{B^-}) for the calculation of ? pKa

(pKa-pKa*) using the following equation.

$$pK_a - pK_a^* = 2.1 \times 10^{-3} (V_{BH} - V_{B^-}) \text{ at } 25^0C$$

Even if the compound is non-fluorescent, this method can make use of absorption maxima for the calculation of ? pKa.

2. **Fluorimetric titration method (pH dependence of fluorescence):**

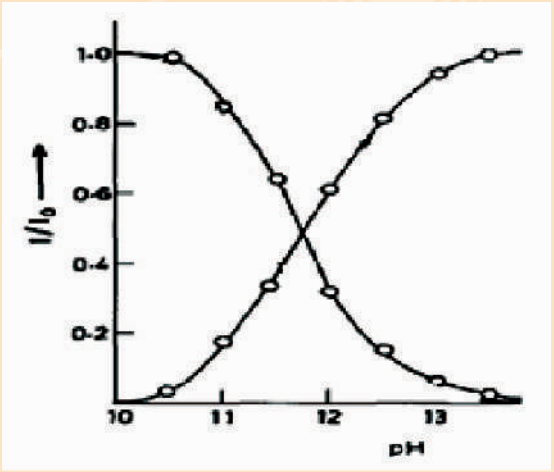


Fig.2. Plot of relative fluorescence intensities of the beta-naphthylamine and its anion Vs pH

Weller developed a method to find out the excited state pKa value using fluorescence intensity as a function of pH of the system. Fluorescence of a molecule depends on the pH, which decides whether the molecule exists as acid or conjugate base in the excited state. Spectrophotometric titration of pH dependence of absorption of an acid and its conjugate base will reveal the ground state pKa value, whereas fluorimetric titration of pH dependence of fluorescence will give excited state pK_a (pK_a^*) value.

$$NNH_2 \overset{pK_a^*(I)}{\rightleftharpoons} NNH^- + H^+$$

It is found that the pK_a^* (I) of 2-Naphrthylamine is 11.75 as revealed by the intersection of curves (Fig.2).

Excited state geometry: Geometry of a molecule, if different from ground state geometry, can be analyzed by the mirror image symmetry of absorption and fluorescence. As seen in figure 3 , mirror image symmetry of Anthracene absorption and emission revealed its same geometry in ground and excited state. But in case of biphenyl molecule, it is non-planar in the ground state and attains planarity in the excited singlet state and this change is shown by the absence of mirror image symmetry of the absorption and fluorescence. (Fig.3).

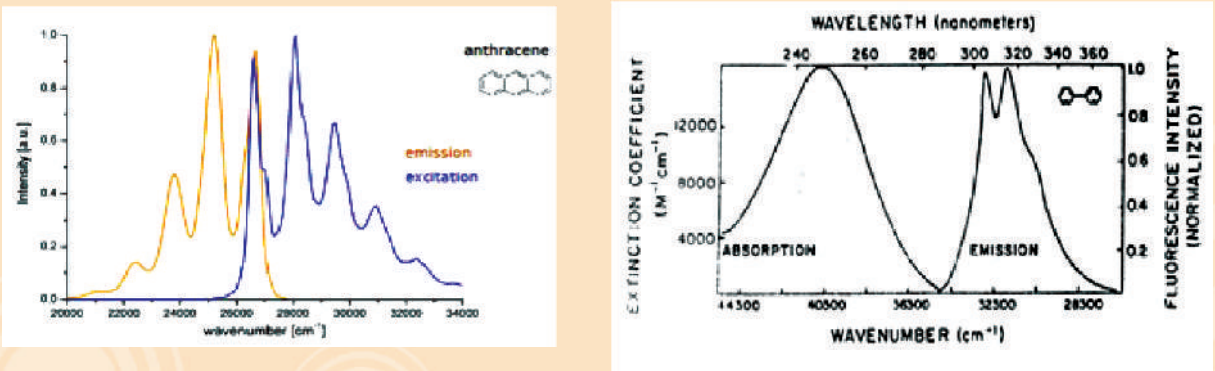


Fig.3. Excitation and emission spectra of Anthracence and biphenyl

Excited state Dipole moment: Dipole moment of a molecule increases in the excited state due to increase in polarity of the molecule. Change in dipole moment ? μ (μ_e - μ_g) can be obtained by Lippert equation (Equation -2), which correlates the stokes shift (? $_a$ - ? $_f$) with dipole moment of fluorophore and solvent parameters(å -dielectric constant and n-refractive index, a - onsagar cavity radius, h – plank's constant) .

$$\nu_A - \nu_F = \frac{2\Delta f}{hc}\frac{(\mu_E - \mu_G)^2}{a^3}, \quad \Delta f = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 - 1} \qquad \text{.....(2)}$$

By using this equation excited state dipole moment of fluorophore can be determined. Fluorescent molecules with large solvotochromic shifts (shifts in absorption and emission maximum of the fluorophore due to polarity of solvents) have been developed for use as fluorescent probes in estimating micro polarity in a micro heterogeneous medium, helping elucidation of protein structure. Some of the Organic molecules, which have significant ? μ values are 2-Aminonaphthalene-6-sulfonate (? μ- 9) and N-phenyl-2-aminonaphthalene (? μ- 20) revealing their excited state dipole moment (μ_e) are 9 and 20 times greater than ground state dipolemoment (μ_g).

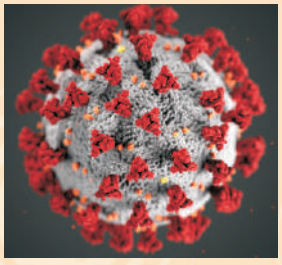
Excited state dimer (Excimer) formation can be identified and analyzed by the variation of fluorescence of a molecule at different concentrations. Florescencecan be used for sensing a number of metal ions by the fluorescence quenching studies. Fluorescence spectroscopy is shown to be a more sensitive and rapid diagnostic tool with high efficiency compared to many routine medical diagnostic tools. It has been applied successfully for the diagnosis of multisystem cancers with high sensitivity and specificity.

The fluorimetric technique was developed only in mid fifties. But today it has wide applications due to its high sensitivity and sophisticated instrumentation. The book on "Principles of Fluorescence Spectroscopy, J.R. LAKOWICZ, Plenum Press, NEW-YORK , with the latest edition by Springer in 2010, is encyclopedic and comprehensive and is recommended without reservation both to the novice(Beginners/Learners) and to the expert in fluorescence."

News, Views and More

Chemistry of Corona Drug Developed by DRDO

The Chemistry of Corona drug developed by DRDO is said to be a big game changer. It is 2-Deoxy-D+Glucose (2-DG) which is to being soon marketed. The hero behind this discovery is said to be the Scientist, Dr. Anil Kumar Mishra who hails from Balia (UP), obtained his M.Sc.(Chemsitry) degree from Gorakhpur University in 1984 and Ph.D degree in 1988 from Banaras Hindu University. His research is mainly based on Molecular Biology and Organic synthesis. After doing the post doctoral research, he has worked as visiting Professor in different foreign countries like France, California (USA) and Max Plank, Germany. He joined DRDO as Sr. Scientist in the year 1997.



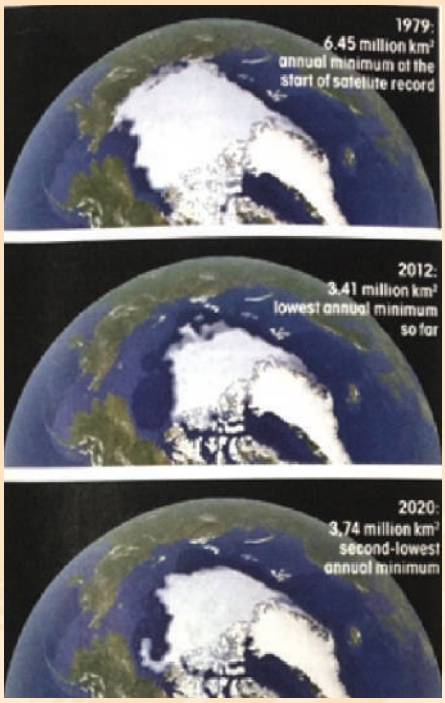
2-DG is a mimic of D-Glucose prepared by replacing -OH group at C2 by H-atom. Hence, the name 2-Deoxy-D-Glucose meaning removal of oxygen from 2nd carbon. Being mimic of D- Glucose, it gets easy passage into the cells where Corona virus is already present.

Glucose breaks down into two three carbon compounds one of them being pyruvate anion (CH3COCOO-) with release of energy. It is a metabolic process called Glycolysis. It is this energy on which all living organism survive. Corona virus also survives on this energy. Unlike D-Glucose, 2-DG is unfit for glycolysis. No energy is evolved. The sustaining of life becomes difficult and as such Corona virus dies within a week in want of energy. It is said that this drug also lowers the oxygen dependence of patients. This drug is also antitumour/anticancer by the same mechanism. If it is able to destroy killer Corona virus, crores of precious lives will be saved. Thank you DRDO.

The science behind the 2DG drug for Covid-19 developed by DRDO: 10,000 doses of 2DG by DRDO had been released to some leading Delhi hospitals! Hopefully, Mass-scale production is ramping up will start soon at Hyderabad and likely at other centers! The principle of operation is very simple: "Cheat the Cheater"! You know that any virus, once inside the body, makes its own copies by cheating our human cells and takes their protein to multiply itself! The brilliant thought process by Indian scientists was simple! For every doubling of virus cell, it needs energy (glucose!). So, the medicine is simply a "Pseudo" Glucose which the multiplying virus intakes but actually, this glucose makes it neuter (unable to multiply!). Thus 'Cheating the cheater' once the rapid multiplication of virus is halted, our own anti bodies can readily combat it and overpower within hours! Simply Geneious! Be proud of Indian scientists!

Arctic on the Ice

No place felt the heat in 2020 like the Arctic and its surrounding seas. Its ice cover melted to its second lowered annual minimum extend of 3.74 million KM^2 in summer, while the freeze-up in autumn saw a sluggish start. The Arctic sea ice minimum is the given day in a year when the ice cap reaches its minimum extent. The lowest annual minimum recorded so far was 3.41 million km^2 in 2012.



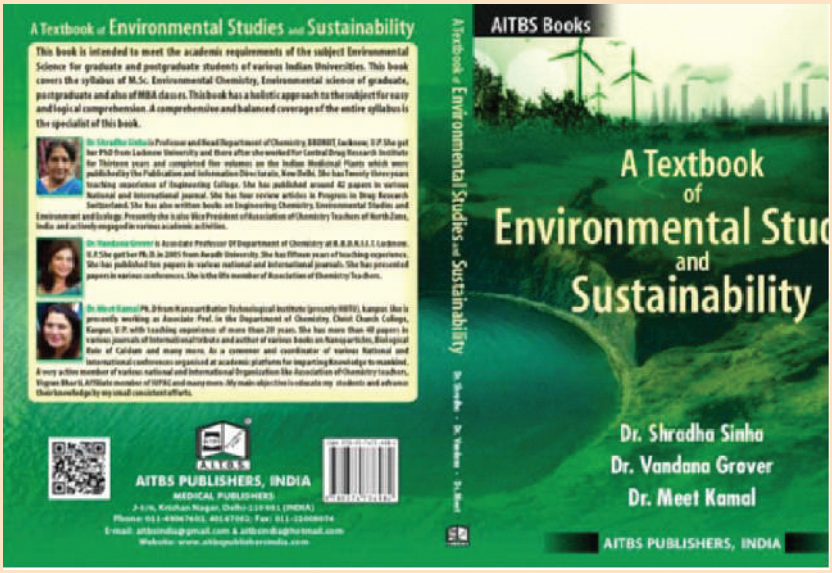
Many notable weather events hit the Arctic in 2020, such as the heatwave over Siberia in the first half of the year, which led to rapid melting of the East Siberian and Laptev Seas. But 2020 was not an exceptional year –antellite data shows about 40 years (1979-2019) of decline in Arctic sea ice. Sea ice decline is strongly linked to global warming and atmospheric carbon dioxide(CO_2) says JullienneStroeve, a polar scientist and professor at the University of Manitoba, Canada, and the University College London, UK. Stroeve and Dirk Notz of the University of Hamburg, Germany, say that for every one tonne of anthropogenic CO2 emissions released into the atmosphere, the Arctic loses 1 m^2 of ice in winter and 3m^2 in summer.

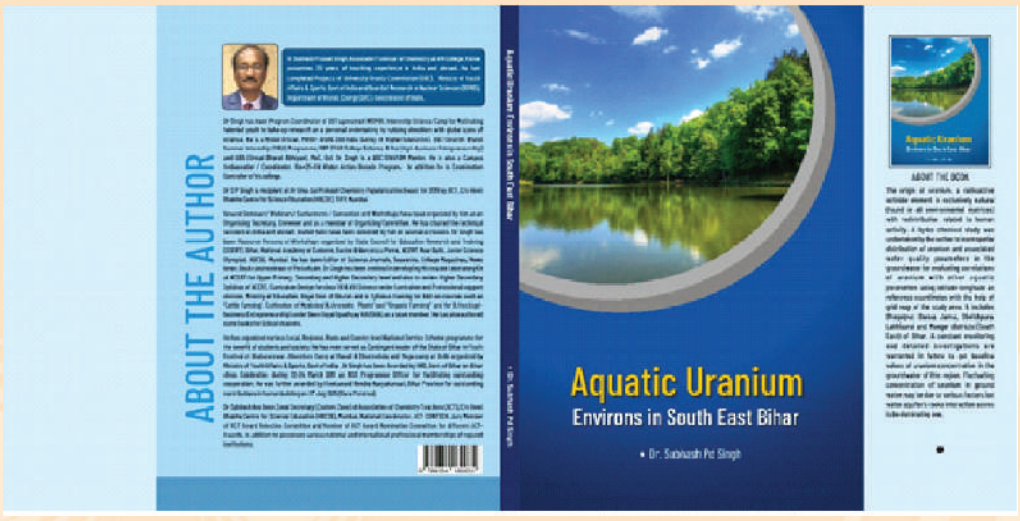
The paper, published in IOP Science, also found that melting seasons are getting longer due to the ice-albedo feedback (melting of the ice leads to a large amount of open water, which absorbs more sunlight and gets warmer). This delays the freezing of the Arctic Ocean-it starts about a week later per decade from 1979. Also the age of the ice is decreasing. In 1979, much of the ice cover was more than four years old, currently, almost all of it is first year ice which forms in the winter but does not survive the next summer.

Arctic Melting will lead to more Global Warming

Jullenne Stroeve, polar scientist, speaks on why we should worry about the rapid decline of the Arctic sea ice. What factors are responsible for the ice-albedo feedback that exte3nded the melting season in the Arctic? The winter Arctic Oscillation (atmospheric circulation pattern above the Northern Hemisphere) was a likely factor in the large amounts of open water in Eurasia this (2020) summer. The earlier melt onset is a result of these changes in atmospheric circulation, which is bringing more warm moist air into the Arctic, whereas delays in the freeze up season are linked to the expanding open water areas in the summer that absorb the sun's energy. The heat they capture has to be released back to the atmosphere before ice can form again.

What does young, fragile ice in the Arctic cover imply in terms of climate change? We have thinner ice now that is easier to melt in summer. The Arctic acts as our planet's refrigerator, and so removing the ice and snow there warms





List of ACT Life Members During January to April 2021

Sr. No.	LM No.	Name	Post
1.	2302	Dr. P. Anbusrinivasan	Assistant Professor
2.	2303	Radika Mahajan	Associate Professor
3.	2304	Dr. Alka Tangri	Associate Professor
4.	2305	Dr. Archana Dixit	Assistant Professor
5.	2306	Dr. Sandip Babarao Ghodile	Assistant Professor
6.	2307	Dr. Meenal Gupta	Assistant Professor
7.	2308	Dr. Ajit Joshi	Associate Professor
8.	2309	Dr. Dimple Kumari	Assistant Professor
9.	2310	Dr. RambabuDandela	Assistant Professor
10.	2311	Avisa Indira	HOD (Chemistry)
11.	2312	Dr. Sreenivasulu Reddymasu	Assistant Professor
12.	2313	Dr. Vinod Kumar Tiwari	Professor
13.	2314	Mr. Ayon Chakraborty	PGT (Chemistry)
14.	2315	Dr. Arun Sharma	Assistant Professor
15.	2316	Dr. Alka Harit	Assistant Professor
16.	2317	Prof. Dr. Kishan Shankarrao Lohar	Professor & Head
17.	2318	Dr. A. Geetha	Associate Professor
18.	2319	Dr. Neha Agarwal	Assistant Professor
19.	2320	Dr. Sunita Singh	Assistant Professor
20.	2321	Dr. Ashutosh Shukla	Professor
21.	2322	Supriya Vyas	Assistant Professor
22.	2323	Dr. Navneeta Upadhyay	Assistant Professor
23.	2324	Dr. M. Bhagiyalakshmi	Assistant Professor
24.	2325	Dr. Sandhya Dixit	Assistant Professor
25.	2326	Dr. ShipraBhati	Assistant Professor
26.	2327	Mr. Keyur Dinesh Bhatt	Associate Prof. & HOD (Chemistry)
27.	2328	Dr. Nisha Garg	Assistant Prof. & HOD (Chemistry)
28.	2329	Mr. Tarun Kush	Vice Principal
29.	2330	Dr. S. Santhisudha	Woman Scientist (WOS- A) - DST
30.	2331	Dr. Nayma Siddiqui	Assistant Professor
31.	2332	Dr. Sanjay Parihar	Assistant Professor
32.	2333	Dr. Mrs. Meet Kamal	Associate Professor
33.	2334	Dr. Shweta Chand	Associate Professor
34.	2335	Prof. Dr. Menka Bhasin	Professor
35.	2336	Dr. Ranjit Kumar	Assistant Professor
36.	2337	Mr. Amooru Gangaiah Damu	Professor
37.	2338	Dr. Archana Jain	Assistant Professor
38.	2339	Dr. Mala Mathur	Professor
39.	2340	Mr. Paladugu Suresh	Assistant Professor

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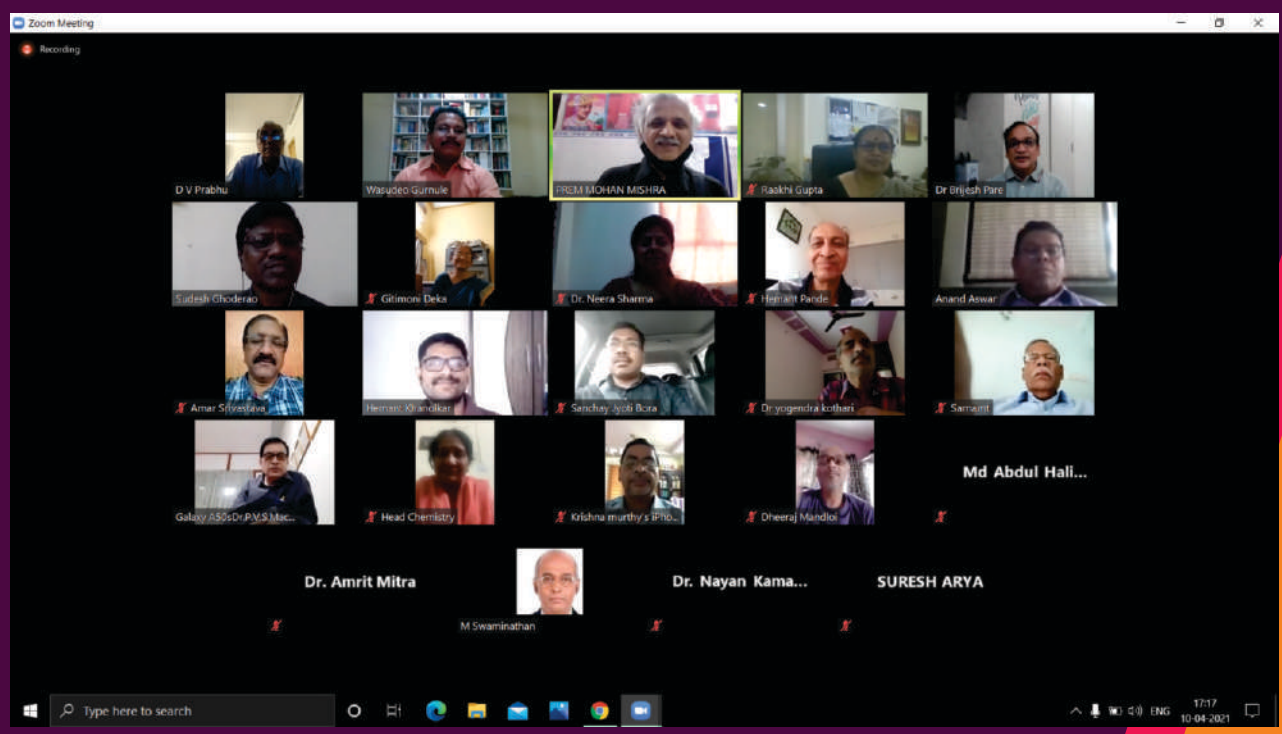

ACT NEWS LETTER

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