



# ISAS newsletter

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ISAS newsletter is a quarterly email publication of Indian Society of Analytical Scientists composed and edited by Dr. V. Babu, Secretary-ISAS Kerala Chapter . He works as Scientific Officer in the R&D Department of Hindustan Insecticides Limited, Udyogamandal, 683501, Kerala State.

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### *Editor's Note:*

Welcome to ISAS News Letter Volume 2, No 1. I wish all our readers a Very Happy and Prosperous 2010. Members of ISAS may kindly send articles for publication in the newsletter. Articles may please be sent to the editor by e-mail. I would like to thank all the contributors for the time and effort they have spent preparing articles for this edition which I hope you will find both informative and interesting.

### **Message from President-ISAS**

*On behalf of ISAS, I wish all our readers a Very Happy and Prosperous New Year.*

This is an exciting time for analytical science. The demand for information about the interrelations of chemical composition – structure - properties for natural and synthetic materials are exploding. Analytical data are requested in the spatial domain from the atomic/molecular scale within biological structures etc. to the scale of global earth observation and in time windows from femtoseconds in laser applications to millions of years for palaeoclimate research . Several production processes have to be controlled by on-line analysis. The rapid development of 'nano' and 'bio' technologies could not have happened without analytical tools. Life-science research is now moving from genomics towards a postgenomic era with transcriptomics, metabolomics and proteomics. The bioanalytical field is expected to play a crucial role. Novel innovative and high-performance bioanalytical techniques provide the means for new applications in medicine and life science. Molecular recognition often occurs at an interface. A particle can be a useful platform for molecular separation and construction of sensing devices. Although interfaces and particles have thus played essential roles in the developments of analytical methodology, analytical scientists have not paid special attention to such aspects when working on macroscopic scales. Recent developments of instrumental measurements have allowed analytical scientists to work on the molecular bases, and nanotechnology provides various materials designed in the micro- to nanometer dimensions. Analytical scientists should open new frontiers by dealing with nanomaterials in proper ways and should facilitate deeper understanding of the chemistry taking place therein through the developments of novel approaches to nano spaces. The aim of innovations in analytical sciences is to create new technologies that allow unknown phenomena or chemical species to be measurable and detectable. There are many phenomena or materials that can be uncovered only by novel analytical technologies. The innovations include the development of analytical tools in relation to topics such as the structure and function analysis of biological matters and the life-related phenomena, the atomic and molecular scale measurements at the surfaces and interfaces, and the environmental and ecosystems analysis. New developments have taken place in the area of sample pretreatments, new analytical reagents, and software.

Recent developments in spectroscopy has greatly encouraged its application to analytical science. One direction of the development of spectroscopy is an extension of wavelength regions. This has brought rapid advancement of vibrational spectroscopy particularly in near-infrared region and Terahertz region. Another direction is progress in imaging, nondestructive analysis, and in-situ analysis. It has facilitated to analysis as it is without destruction. Meanwhile, there have been great strides made in the studies of Raman spectroscopy, for example, like femtosecond time-resolved spectroscopy, CARS microscopy, near-field Raman spectroscopy and SERS. New spectral analysis methods, and new applications to analytical chemistry for near-infrared, infrared, Terahertz, and Raman spectroscopy provide new tools to analytical scientists.

There is no shortage of exciting problems for analytical scientists in many areas, both with cutting-edge scientific dimensions and with high societal and economic relevance. However, there are awareness issues both within the analytical scientist community and with respect to the perception by scientists from other disciplines, and also by regulators, the media, the public etc. Analytical scientists are now able to predict the near future advances of analytical chemistry in a number of general directions, among them are the further pushing of performance limits of analytical methods (such as smaller 'target' sizes to achieve high spatial resolution, faster analysis for real-time or high-throughput data), simultaneous multi-parameter analysis of increasingly complex systems (living organisms, ecosystems, etc.) including their non-target screening, progress of non-invasive methods, provision of "sustainable" analytical data with demonstrated reliability (both precision and trueness) which are fit for the purpose of making qualified decisions. Moreover, the miniaturisation of devices, laboratory automation and on-line process analysis are likely to continue as trendsetters. Above all the abilities of well trained and continuously updated analytical scientists to combine their specific competences with interdisciplinary approaches in a problem-solving oriented manner will provide analytical science a bright future in the coming decade.

Thank you

Dr VR Nair  
President-ISAS

## **Indian Analytical Science Congress -2009 (IASC-2009)-A Report**

The Indian Analytical Science Congress 2009 (IASC -2009) was organized by the Indian Society of Analytical Scientists (ISAS) at the Silver Hills Resort, Lonavala, Maharashtra State during November 12-13, 2009. The theme of the congress was „ Analytical Science for Industrial Development and Technological Progress“. This Conference was conceptualized based on the demand for a platform where leading analytical scientists, academicians, researchers, business leaders, policy makers and other stakeholders would be able to interact, exchange ideas and communicate with each other on all aspects of the niche areas of analytical science to face the challenges of globalization and its opportunities for economic growth in our country. The conference covered almost all the fields of analytical chemistry. From analytical atomic spectrometry and nuclear analytical methods to nano-technology, separation science, and sensors of all kinds, the symposia and posters painted a broad canvas of the present state of the art in analytical science, and also suggested future directions and dreamed about future capabilities.

Around 100 research papers have been received from academia and industry. This Conference was continuation of the series established by the ISAS in 2007 when IASC - 07 was held in Nagpur. This was the first analytical science congress organized by ISAS and was a successful challenge. Then, IASC -08 took place in Munnar, Kerala in 2008 and the latest IASC-09 in Lonavala, Maharashtra in 2009. These events provided adequate scientific and social environment for local scientists to discuss new developments in the field of analytical science, share experiences and results with experts.

### **Inaugural Session**

Dr L.M. Gantayet, Associate Director, Beam Engineering and Technology Development Group Bhabha Atomic Research Centre, Trombay, Mumbai inaugurated the Conference. He spoke on the application of analytical science in nuclear technology and described how analytical procedures were scaled up to produce some of the valuable isotopes used in the nuclear industry. He also discussed several areas in Nuclear Technology where analytical techniques play a key role. Prof. R. T. Sane, Hon. Director, Guru Nanak Institute of Research and Development, Matunga, Mumbai-400 019 in his key note address on Analytical Problems and Prospects in Determining biosimilar drugs described various aspects of bioanalytical method and validation, reference standards, endogenously existing compounds, protein binding,, common instrumental techniques used, immunoassay, selectivity, matrix effects, etc in the determination of biosimilar drugs. He also discussed the major issues that need to be considered while identifying strategies to evaluate biosimilar drugs. This include a) the ability to detect differences in structure and impurity profile using physico-chemical and biological methods, b)the extent and relevance of non clinical and clinical data required to support similarity, and c)the potential impact of immunogenicity. This approach requires an integration of knowledge from various disciplines including protein chemistry, analytical science, etc. He concluded by saying „ even if the biosimilars are cost saving, they should not push patients towards therapeutic failure with unidentified risk of long term and short term safety concerns. Studies comparing the original and biosimilar products are to be carried out. These studies should demonstrate that there are no meaningful

differences between the biosimilar and the reference biopharmaceutical product in terms of safety or efficacy. Dr V.R. Nair, President-ISAS presided over the function. Chairman of the local organizing Committee Shri Devraj Aiyer, welcomed the gathering. Dr P.P. Chandrachoodan, Programme Officer of BRNS released the book of abstracts. Dr K.K. Abdul Rashid. Hon. Secretary ISAS and Convener of the National Organizing Committee proposed the vote of thanks.



*Dr L.M.Gantayet ,Associate Director, Beam Engineering and Technology Development Group Bhabha Atomic Research Centre delivering the inaugural address of IASC 2009.*

After the inaugural session was followed by technical session I. The technical session I was chaired by Dr P.N.Mohandas, formerly Deputy Director, NIIST, Thiruvananthapuram. The first paper was presented by Dr V. Balaram of National Geophysical Research Institute, Hyderabad. The title of his talk was, ICP-MS, Recent Technological Advances, Applications and Future. During the last 25 years, ICP-MS has become a comprehensive analytical technique which revolutionized elemental analyses and has been widely accepted as a powerful tool for trace and ultra-trace elemental and isotopic analysis of most elements, from lithium through uranium, in a variety of materials. In his presentation he has described the recent advances in ICP-MS for speciation analysis and how this technique has helped to understand the toxicity and bioavailability of arsenic in different compartments of our environment. Finally he concluded that these advances in ICP-MS will have a greater impact on future studies in different branches of Science and Technology. The second invited paper was presented by Dr S.V.Godbole, Head, Spectroscopy section, Radiochemistry Division, Bhabha Atomic Research Centre, Trombay. The title of the paper was ,Recent Investigations in AAS: Matrix Effects in GFAAS and Development of ICP-AAS.

Two major problem encountered in GF-AAS technique are (i) severe suppression in the absorbance for the majority of analytes in the presence of U/Pu/Th/Zr matrices in comparison to simple aqueous solutions and (ii) the technique is not suitable for refractory and carbide forming elements. Dr Godbole presented the efforts that have been directed to understanding these matrix effects and developing an AAS unit using ICP as atomizer (ICP-AAS) so that it will enable atomization of refractory elements. For understanding matrix effects in GF-AAS, studies have been carried out by him and his team to identify the changes in surface morphology, and the elements and compounds formed on surface using SEM, EDAX and XRD techniques in addition to GF-AAS measurements. In the case of ICP-AAS, since commercial units are not available, such a unit was designed and assembled in BARC. The salient features of these investigations were discussed. The third invited paper was presented by Dr A.G. Page, Consultant, Metallurgical Services, Mumbai. The methods developed and used for day-to-day analysis for compositional characterization of various types of steels, copper base alloys, etc. were described by Dr Page. He also presented the data obtained from the analysis of some of these matrices and efforts made to establish utility of such an approach in ICP-AES.

The title of the fourth invited talk was, "HPTLC in food analysis: Special emphasis on analysis of food additives, contaminants and mycotoxins". The paper was presented by Dr. Prem Kumar Jaiswal, Former Director of Laboratories, Central Agmark Laboratories, Govt. of India. In his presentation he described the application of HPTLC for detection/determination of food additives, aflatoxin, mycotoxins, major contaminants in foods at the lowest level using HPTLC. HPTLC is a versatile technique with wide application in food, drug, cosmetics, herbal etc. According to Dr Jaiswal the technique of HPTLC is simple, cheap, convenient and suitable for screening large number of samples simultaneously.

In the Session II four invited talks were presented. The first invited talk was presented by Prof. Deqing Zhang, Beijing National Laboratory for Molecular Sciences, Organic Solids Laboratory, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100080, China. The title of his talk was, "New Organic Functional Molecules for Chemo/Bio sensors". In this presentation, Prof. Deqing Zhang first described some new tetrathiafulvalene (TTF) molecules for chemical sensors, by making use of the unique feature of TTF (and its derivatives), which can be reversibly transformed into the radical cation  $TTF^{•+}$  and dication  $TTF^{2+}$  through either chemical or electrochemical oxidations at easily accessible potentials. These include chemical sensors towards  $O_2$ ,  $Hg^{2+}$ , saccharides based on TTF-anthracene dyads. In addition, he also introduced new chemo-/biosensors including DNA detection method and label-free fluorescence nuclease assay based on the aggregation-induced enhanced emission (AIE) of silole. Dr A. Ajayaghosh, Photosciences and Photonic Group, Chemical Sciences and Technology Division, National Institute for Interdisciplinary Science and Technology (NIIST), CSIR, Trivandrum presented the next invited talk on, "Rational Design Of Molecular Probes For Biologically Relevant Analytes". Dr Ajayaghosh and his group are engaged in developing fluorophores, useful for the selective detection of biologically important cations and neutral molecules. With this objective, recently they have exploited squaraine dyes, a class of organic dyes for the design of molecular sensors. Subsequently, he has reported a novel strategy for the detection of total aminothiol content in human blood plasma using a near infrared absorbing squaraine dye which is

sensitive to thiol attack. Details of these studies were presented by him during the invited talk.

Dr. M. Jayakannan, Department of Chemistry, Indian Institute of Science Education & Research (IISER), SAI Trinity Building, Pune 411008 gave the next invited talk on, "The Role of Modern Analytical Approaches in Template Assisted Conducting Polymer Nano materials." During the course of development of conducting polymer nano materials, he has put significant efforts to understand the molecular interaction in the templates using modern analytical spectroscopic tools such as dynamic light scattering, high resolution electron microscopes, NMR, FT-IR and Wide angle X-ray diffractions to trace the mechanistic aspects of these template-assisted synthetic process. The synthesized nano-materials were also employed as sensor for chemical and biological substances. The presentation focused on the recent developments in the above topic and also demonstrated the need for the systematic analytical approaches for sustainable nano materials research. The last paper in the Session II was delivered by Dr P. Sudhadevi of Central Glass and Ceramic Research Institute, Calcutta. The title of her talk was, "Size Effects in Semiconducting Gas Sensors: Some New Insights. Her talk covered an overview of the processing, characterization fabrication and properties of a few selected oxides such as SnO<sub>2</sub> and CeO<sub>2</sub> and their gas sensing characteristics. Work carried out at CGCRI on for fabricating sensors from nano particles for detecting butane, hydrogen and sulphur dioxide gas were presented. The importance of using nano particles of oxides for developing gas sensors with higher selectivity and sensitivity were presented with selected examples. This was followed by poster session in which 66 posters were presented.

The technical programme on 13<sup>th</sup> November started with Poster Session. Technical Session III started at 9.00 AM. This was chaired by Dr M. Mohapatra, Radiochemistry Division, Bhabha atomic Research Centre, Mumbai. The first invited talk in Session III was presented by Dr M.L.P Reddy of NIIST, Thiruvananthapuram. He spoke on, " Tuning of Emission Colors with lanthanide Complexes: Facile Photoluminescent Production of True White Light". It was demonstrated that with judiciously chosen red- (Eu<sup>3+</sup>, Pr<sup>3+</sup>, Sm<sup>3+</sup>), green- (Tb<sup>3+</sup>, Er<sup>3+</sup>) and blue-emissive (Tm<sup>3+</sup>, Pr<sup>3+</sup>, Ce<sup>3+</sup>, Dy<sup>3+</sup>) ions doped in a suitable host, it is possible to obtain phosphors which emit across the entire visible spectrum with high color purity. He reviewed some of the seminal work in the area, along with new developments in the field. In their laboratory, they have demonstrated a facile molecular approach to generate white light emission by combining carboxylic functionalized poly(m-phenylenevinylene)s polymeric architectures with lanthanide β-diketonate complexes. This work was also presented by Dr Reddy. "Electron Microscopy: An Inevitable Tool for Materials Characterization", was the title of the next invited talk by Dr Peter Koshy, Head, Electron Microscopy, Materials and Minerals Division, National Institute for Interdisciplinary Science and Technology (NIIST), CSIR, Thiruvananthapuram-695 019. In his presentation he stressed the importance of Electron Microscopy and Energy Dispersive Spectroscopy in the multidisciplinary areas of material research in chemistry, biochemistry, environmental and energy science, material science and medical science. Dr Koshy's talk provided vital know-how of the ground rules for getting the best microstructure and to bring in the concepts of the most efficient and robust approach to analyze materials by Energy Dispersive Spectroscopy. Pranav M. Nagarnaik, Environmental and Water

Resources Division, Zachry Department of Civil Engineering, Texas A&M University, College Station, TX, USA presented the next invited talk on Analysis and Environmental Loading of Pharmaceutical and Personal care Products from Healthcare Facility Waste Water using Selective Ion Extraction and UPLC-Tandem Mass Spectroscopy. Presence of Pharmaceuticals and Personal Care Products in the wastewater effluents and potable supplied water has increased the need to develop a method to identify these emerging contaminants at their sources. A rapid selective solid phase extraction followed by ultra performance liquid chromatography in combination with triple quadrupole mass spectrometric (UPLC - MS/MS) method was used by their team for detection of 48 pharmaceuticals and 6 metabolites in the healthcare facilities wastewater. Fifty four pharmaceuticals were distributed across 9 of the 14 therapeutic categories from Anatomical Therapeutic Chemical (ATC) classification system. Their findings provide a basis for future research needed for risk management from pharmaceutical sources to the environment.

Session IV was chaired by Dr S. Sugunan, Professor, Department of Applied Chemistry, Cochin University of Science and Technology. Dr. Ajit Datar, Shimdazu Analytical (India) Pvt. Ltd. Mumbai presented the first invited talk . In his lecture the following aspects were covered:

a)The History of development of LC-MS especially in developing interface between LC and MS, b)The current Interface technologies: Atmospheric Pressure Ionization (API), (c)Mass Spectrometers used in LC-MS applications(c)The concept of Tandem Mass Spectrometry, (d)The Use of Triple Quadrupole Mass Spectrometer, Tandem MS (LC-MS/MS), (e)Hybrid Tandem Mass Spectrometry with LC and its applications. (f)The Applications of LC-MS in Pharmaceutical and biotechnology fields. The second invited talk in this session was delivered by Dr S.C.Tripathi, Fuel Reprocessing Division, Bhabha Atomic Research Centre. The title of his presentation was Gas Chromatography-Mass Spectrometry(GC/MS): Emerging Vistas of the Applications. Dr Tripathi in his talk discussed Applications of GC-MS in Drug detection, explosives/arson investigation, Environmental analysis, Food technology Forensic science, etc. Application of this technique in airport security to detect substances in luggage or on human beings were also discussed. It is becoming the tool of choice for tracking organic pollutants in the environment. For most organic analysis of environmental samples, including many major classes of pesticides, it is very sensitive and effective. In combination with isotopic labeling of metabolic compounds, the GC-MS is used for determining metabolic activity. The Role of Advanced LCMS as an Active Analytical Technique was the topic of invited talk presented by Dr Abhijeet Kanungo, Agilent Technologies India Pvt. Limited ,Mumbai. In his presentation Dr Abhijeet Kanungo presented the practical use and growing potential of this technique. The main strategies for achieving the best sensitivity in any condition and with any molecule was presented. The presentation also covered small molecule and proteomics applications of LCMS in comparison to the conventional techniques used today. In addition to these invited talks there were ten oral presentations on Neutron activation analysis, Inductively Coupled Plasma Atomic Emission Spectrometry, Energy Dispersive XRF, Separation by solvent extraction, Characterization of nuclear fuel, Thermal analysis, etc. There were a few presentations by vendors of analytical instruments.

### *Poster Session*

The wealth of material covered at the poster sessions was remarkable. Among many significant contributions, two works were selected for the best poster awards. Mr. Sivaramapanicker Sreejith, Photosciences and Photonics Group, Chemical Sciences and Technology Division, National Institute for Interdisciplinary Science and Technology (NIIST), CSIR, Trivandrum, India-695019 was awarded Prof. B. C. Haldar Memorial award for the poster entitled "Estimation of Total Aminothiol in Blood Plasma using Molecular Probe" and Dr K.K. Majumdar Memorial award was presented to Mr S.J. Richard Prabakar, Department of Analytical Chemistry, School of Chemical Sciences, University of Madras, Guindy Campus, Chennai, TamilNadu-600 025 for his poster entitled, " CuHCF Surface modified graphite Sol-Gel Ceramic Electrode and its Application for Simultaneous Determination of Benzenediols".

The concluding session was chaired by Dr AVR Reddy, Head, Analytical Chemistry Division, Bhabha Atomic Research Centre. Dr Reddy spoke on the importance of Analytical Science in all important areas of our day to day life. Analytical Chemistry is also an integral part of the nuclear energy programme and plays a crucial role in materials characterization and quality assurance. In fact, one of the first chemistry activities in the saga of the Indian atomic energy programme, was the analysis of minerals for the exploration and estimation of uranium. Since then, analytical chemistry has become an integral part of the Indian nuclear energy programme. Apart from these analytical chemistry plays an important role in the development of new and advanced materials for various applications in the nuclear industry. With the Indian nuclear energy programme poised to make greater strides in terms of enhanced power production and adopting diverse advanced reactor concepts, analytical chemists will be called upon to play even greater roles. Dr Reddy said ISAS should initiate various programmes for the promotion of Analytical Science in our country.



A view of the participants of ISAC 2009

There was a feed back session in which the participants voiced their opinions and comments. All those who attended the Lonavala conference agreed that the event was a great success. There was record attendance at the technical sessions, and the sessions showed the wide range of areas covered by Analytical Chemistry.

Overall, IASC-2009 resulted in a lively interdisciplinary conference where research and development efforts and emerging issues in the area of analytical science were thoroughly discussed in a enjoyable atmosphere. The conference was well organized and managed throughout, and prompted optimum interaction between the delegates. An interdisciplinary conference of this kind has the advantage of the cross-fertilization that occurs when people dealing with various aspects of analytical chemistry come together and discuss diverse ways of looking at similar problems. The diversity and depth of study reported was truly impressive . The success of this conference led to the decision to hold an international conference on Analytical science at Cochin during 2010.

**Proceedings of the IASC 2009 Part-I is given below:**

# INDIAN ANALYTICAL SCIENCE CONGRESS - 2009

Theme-Analytical Science for Industrial Development and Technological Progress

Organized by : Indian Society of Analytical Scientists (ISAS)



November 12-13, 2009

LONAVALA-MAHARASHTRA



## MESSAGE FROM PRESIDENT - ISAS

On behalf of the Indian Society of Analytical Scientists (ISAS), I sincerely welcome you to attend the Indian Analytical Science Congress 2009. The Indian Society of Analytical Scientists was started in 1983 by a group of visionaries from Bhabha Atomic Research Centre, Mumbai. Today it is one of the oldest and most prestigious professional associations in India.

The ISAS is now spread throughout the country with more than two thousand life members and thirteen chapters. This year is our 26th anniversary. ISAS is very honored that you could join us for this milestone event. The theme for the Indian Analytical Science Congress this year is "Analytical Science for Industrial Development and Technological Progress." The year 2009 has been a very challenging year indeed. Natural disasters, the energy crisis, and the financial market turmoil relentlessly hit the world one after another and threaten world prosperity. More than ever, the world needs young and dedicated scientists and engineers to beat the odds and accomplish more for less. For example, we need new technologies for increasing industrial production; we also need new technologies for better health care when public budgets are tight; above all, we certainly needs better technology for increasing agricultural production, and regain sustainable prosperity.

At this congress, we will therefore discuss and present the application and future technology trends of analytical science in the areas of industrial development and Technological progress. For the two day conference, we have invited many distinguished experts to be our speakers and panelists for the technical sessions and the forum. There are keynote , plenary, invited and contributory papers, posters and award presentations.

During 2008 and 2009, with the unswerving support of many long-time ISAS friends, we have sponsored several activities for our members. These include a tutorial workshop to benefit local professionals, and a picnic for networking among the members. We have continued to work with students from various universities in the country .They need your support and dedication to help them grow and prosper. On closing, I would like to express my deep appreciation to our congress planning committee and financial sponsors for their hard work and generosity. I would also like to thank all the participantsfor attending our third annual congress, and invite you to join our association and participate in our future activities. I believe you will find the ISAS experience very rewarding because it will enhance not only your career future but also broaden your horizons beyond classrooms and laboratories. I wish you all a great conferencing and happy networking!

I hope the proceedings of the conference will be beneficial to the participants in understanding the application of analytical science in industrial development and technological progress and go a long way in promoting analytical science in this part of the country.

Sincerely,  
(Sd)  
Dr V.R. Nair  
President, ISAS

## Preface

It is a great honor and personal privilege for us to organize the Third Analytical Science Congress (IASC 2009) at Lonavala, Maharashtra during 12 -13 November 2009. The theme of this congress is Analytical Science for Industrial Development and Technological Progress. The choice of Lonavala as a venue was especially appropriate in view of its proximity to the chemical industrial capital of India. The flora and fauna will provide an extra dimension to the atmosphere of the conference. The aim of IASC -2009 is to support the scientific research of analytical scientists in the Indian sub continent by inviting the participation of leading analytical scientists from all over the country. Over the last 25 years the India has significantly increased its profile in chemistry, particularly in analytical chemistry. The growing role of analytical chemistry and the contributions of the chemical and pharmaceutical industries to science are significant. The next decade will witness more momentous achievements in analytical chemistry as well as its application in different fields for the benefit of mankind in terms of healthy, productive, long , and comfortable life. The main goal of our Conference is to bring together experts from universities, academia, research centres, various laboratories and industry on a national scale, to summarize the current progress in different areas of spectroscopy and to stimulate contacts and mutual exchange of experience and ideas. The emphasis is put not only on presentation of the latest scientific achievements, new technologies, and instrumentation but also on the applications and utilization of analytical science in different fields of practical life. The Conference also provides a possibility to get acquainted with new instrumental techniques, spectroscopy equipment, laboratory materials and instruments, reference materials, science literature, etc. which are exhibited by several distribution companies.

We particularly thank the participants who are contributing scientific papers as oral and poster presentations at this conference. With the participation of the India's leading scientists from 22 states, This conference will give a good opportunity for all participants to access recent information on achievements in analytical sciences as well as to share and exchange their experiences during the conference.

This year Conference offers a 2 days scientific program consisting of plenary lectures, invited lectures, session lectures, oral presentations, and poster presentations. The topics covered includes Bio-analytical Chemistry, Electro-analytical Chemistry, Thermal Analysis, Atomic and Molecular Spectroscopy, Mass Spectrometry, Separation Science, Sampling and Sensor Technology, Miniaturization Technology , Environmental Analysis, Food and Drug Analysis, Materials Analysis .The conference is being attended by participants . The participation of a large group of active young Indian analytical chemists is made possible by the financial support of the Board of Nuclear Sciences, Department of Atomic Energy.

I hope that this Conference will provide a great opportunity for developing new cooperative projects, new personal collaborations or exchanges, and many fruitful ideas for the advancement of Analytical Science. I wish all of you a very enjoyable stay here in Lonavala and I hope that despite the rather busy schedule you will get time to enjoy the natural beauty of this hill station and able to visit some of cultural, historical, and natural monuments for which the Lonavala /Khandala region is unusually rich.

The organizing committee wish to place on record our thanks to BRNS, CSIR, DST for providing funds to organize this conference, I also thank the members of the national advisory committee and national organizing committee for their contributions to make this conference a great success. I am also thankful to all organizations who have contributed advertisements , participated in the exhibition and those who have sponsored local hospitality. My special thanks are due to those persons working in the back stage looking after every small detail particularly members of the local organizing committee.

Devraj Aiyer  
Chairman-Local Organizing Committee

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Government of India,  
Mumbai.**

**Council of Scientific and Industrial Research (CSIR),  
Government of India , New Delhi**

**Department of Science and Technology (DST),  
Government of India, New Delhi**

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### **IT-01 ICP-MS, RECENT TECHNOLOGICAL ADVANCES, APPLICATIONS AND FUTURE**

**V. Balaram**

National Geophysical Research Institute (Council for Scientific and Industrial Research),  
Uppal Road, Hyderabad - 500 606

### **IT-02 NEW ORGANIC FUNCTIONAL MOLECULES FOR CHEMO/BIOSENSORS**

**Deqing Zhang, Guanxin Zhang, Ming Wang, Lei Liu, Lihua Peng, Daoben Zhu**

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### **IT-03 RATIONAL DESIGN OF MOLECULAR PROBES FOR BIOLOGICALLY RELEVANT ANALYTES**

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### **IT-04 TUNING OF EMISSION COLORS WITH LANTHANIDE COMPLEXES: FACILE PHOTOLUMINESCENT PRODUCTION OF TRUE WHITE LIGHT**

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### **IT-05 HPTLC IN FOOD ANALYSIS: SPECIAL EMPHASIS ON ANALYSIS OF FOOD ADDITIVES, CONTAMINANTS AND MYCOTOXINS**

**Dr. Prem Kumar Jaiswal\* Ph.D., D.Sc., F.I.C.**

Former Director of Laboratories, Central Agmark  
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### **IT-06 ELECTRON MICROSCOPY: AN INEVITABLE TOOL FOR MATERIALS CHARACTERIZATION**

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Interdisciplinary Science and Technology (NIIST), CSIR, Thiruvananthapuram-695 019

### **IT-07 ANALYSIS AND ENVIRONMENTAL LOADING OF PHARMACEUTICAL AND PERSONAL CARE PRODUCTS FROM HEALTHCARE FACILITY WASTE WATER USING SELECTIVE ION EXTRACTION AND UPLC -TANDEM MASS SPECTROSCOPY**

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**IT-08 RECENT INVESTIGATIONS IN AAS : MATRIX EFFECTS IN GFAAS and DEVELOPMENT OF ICP-AAS**

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**IT-09 THE ROLE OF MODERN ANALYTICAL APPROACHES IN TEMPLATE ASSISTED CONDUCTING POLYMER NANOMATERIALS**

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**IT-10 ICP-AES AS APPLIED TO METALLURGICAL INDUSTRY**

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**IT-11 HYPHENATED TECHNIQUES: LC-MS**

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Makwana Road, Marol, Andheri (E.), Mumbai – 400 059, India.

**IT-12 GAS CHROMATOGRAPHY-MASS SPECTROMETRY (GC/MS): EMERGING VISTAS OF THE APPLICATIONS**

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**IT-13 GAS CHROMATOGRAPHIC DETERMINATION OF MONOMERS IN THE ACRYLIC COPOLYMER EMULSION**

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**IT-14 SIZE EFFECT IN SEMICONDUCTING GAS SENSORS : SOME NEW INSIGHTS**

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**CP-01 ION CHROMATOGRAPHY DETERMINATION OF ANIONIC IMPURITIES IN CESIUM IODIDE**

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**CP-02 INVESTIGATIONS OF SPECTRAL INTERFERENCE OF AMERICIUM DURING TRACE ANALYSIS OF PLUTONIUM BY ICP-AES**

**Arijit Sengupta, V.C. Adya, and S.V. Godbole**

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**CP-03 EFFECT OF SAMPLE CONTAINERS ON THE EDXRF DETERMINATION OF U IN AQUEOUS SOLUTIONS**

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**CP-04 DIRECT DETERMINATION OF GALLIUM IN (U-Ga) MIXED OXIDE USING ENERGY-DISPERSIVE X-RAY FLUORESCENCE SPECTROMETRY**

**P.J.Purohit, V.Natarajan, N.K.Porwal, Neelam Goyal, S.V.Godbole and V.K.Manchanda**

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**CP-05 DETERMINATION OF Se, As, Pb, In AND Hg IN AQUEOUS SOLUTIONS USING EDXRF**

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**CP-06 EFFECT OF URANIUM AND/OR THORIUM ON THE EDXRF DETERMINATION OF ZIRCONIUM IN AQUEOUS SOLUTIONS**

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**CP-07 ESTIMATION OF TOTAL AMINOTHIOL CONTENT IN BLOOD PLASMA USING A MOLECULAR PROBE**

**Sivaramapanicker Sreejith and Ayyappanpillai Ajayaghosh\***

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**CP-08 SYNERGISTIC EFFECT ON LANTHANIDE/ACTINIDE SEPARATION WITH CYANEX 301 USING HOLLOW FIBRE SUPPORTED LIQUID MEMBRANE TECHNIQUE**

**A. Bhattacharyya, S.A. Ansari, P. Kandwal, P.K. Mohapatra and V.K. Manchanda**

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**CP-09 EFFECT OF ORGANIC DILUENT ON THE TRANSPORT OF Am(III) ACROSS TODGA BASED SUPPORTED LIQUID MEMBRANES**

**S. Panja<sup>1</sup>, P.K. Mohapatra<sup>2</sup>, S.C. Tripathi<sup>1</sup>, S.K. Munshi<sup>1</sup>, P.K. Dey<sup>1</sup> and V.K. Manchanda<sup>2</sup>**

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**CP-10 DETERMINATION OF IMPURITIES IN HIGH PURITY AMERICIUM MATRIX BY NEUTRON ACTIVATION ANALYSIS**

**Arijit Sengupta, V.C.Adya, R. Acharya, P.K.Mohapatra, S.V. Godbole and V.K.Manchanda**

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**CP-11 SEPARATION OF  $^{90}\text{Y}$  FROM  $^{90}\text{Sr}$  USING A TODGA SORBED EXTRACTION CHROMATOGRAPHY RESIN MATERIAL**

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**CP-12 AN ICP-AES METHOD FOR THE DETERMINATION OF CESIUM AND RUBIDIUM IN DISSOLVER SOLUTION OF SPENT PHWR FUEL**

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**CP-13 ESTIMATION OF COPPER IN COPPER NITRATE SOLUTION USING WAVELENGTH DISPERSIVE X-RAY FLUORESCENCE SPECTROMETER**

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**CP-14 PRECIPITATION BEHAVIOUR OF IMPURITIES IN NUCLEAR GRADE ZIRCONIUM OXIDE**

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**CP-15 QUANTITATIVE ANALYSIS OF IMPURITIES AT TRACE LEVEL IN SELENIUM BY INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY (ICP-OES)**

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**CP-16 RELEVANCE OF CLASSICAL METHODS IN MODERN ANALYTICAL ERA**

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**CP-17 STUDIES ON THE CURE KINETICS AND MASS TRANSFER MECHANISM OF EPOXY- CYANATE ESTER CO-CURED BLEND SYSTEM USING DIFFERENTIAL SCANNING CALORIMETRY IN COMBINATION WITH FOURIER TRANSFORM INFRA RED SPECTROSCOPY**

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**CP-18 RECOVERY OF RADIO-CESIUM USING CALIX-CROWN-6 ETHER:  
STUDIES WITH DILUTED HLW**

**P. K. Mohapatra<sup>1</sup>, P.S. Dhama<sup>2</sup>, S. Panja<sup>2</sup>, P. Jagasia<sup>2</sup>, S.C. Tripathi<sup>2</sup>, P.K. Dey<sup>2</sup> and V. K. Manchanda<sup>1</sup>**

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**CP-19 STUDIES ON THE RELATIONS BETWEEN COAL ASH YIELD AND ITS  
CHEMICAL COMPOSITION**

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**CP-20 NATURAL RADIOACTIVE DISEQUILIBRIUM IN URANIUM ORES AND  
SOILS FROM THE SINGHBHUM SHEAR ZONE, EASTERN INDIA**

**A. Chakrabarty Patra, S. Mohapatra, S. K. Sahoo, R. H. Pillay, R. M. Tripathi  
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**CP-21 APPLICATION OF ENANTIOSELECTIVE TECHNIQUE FOR  
SIMULTANEOUS ESTIMATION OF SIBUTRAMINE AND ITS ACTIVE  
METABOLITES IN HUMAN PLASMA BY LIQUID CHROMATOGRAPHY-  
ELECTROSPRAY IONIZATION TANDEM MASS SPECTROMETRY**

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**CP-22 CHEMICAL EVALUATION OF TAMRA BHASMA**

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**CP-23 SOLID-LIQUID EXTRACTION OF MIXTURE OF HEAVY RARE-EARTHS  
FROM PHOSPHORIC ACID SOLUTIONS USING TULSION CH-96**

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**CP-24 STUDIES ON SEPARATION AND RECOVERY OF PALLADIUM AND  
PLATINUM FROM CHLORIDE LEACH LIQUORS OF SPENT AUTOMOBILE  
CATALYST**

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**CP-25 SEPARATION FACTORS DETERMINATION OF DIVALENT COBALT AND NICKEL FROM SULPHATE SOLUTIONS WITH TOPS 99 AS EXTRACTANT AND CYNEX 471 X ACTING AS SYNERGIST**

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**CP-26 AMPEROMETRIC SENSOR FOR THE DETERMINATION OF HYDRAZINE BASED ON NICKEL HEXACYANOFERRATE MODIFIED ELECTRODE FABRICATED THROUGH A NEW ROUTE**

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**CP-27 GNP-NiHCF PARAFFIN WAX COMPOSITE MODIFIED ELECTRODE FOR THE DETERMINATION OF L-DOPA**

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**CP-28 CuHCF SURFACE MODIFIED GRAPHITE SOL-GEL CERAMIC ELECTRODE AND ITS APPLICATION FOR SIMULTANEOUS DETERMINATION OF BENZENEDIOLS**

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**CP-29 AMPEROMETRIC SENSOR BASED ON FERROCENE-MODIFIED MULTIWALLED CARBON NANOTUBE NANOCOMPOSITES AS ELECTRON MEDIATOR FOR THE DETERMINATION OF L-CYSTEINE**

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**CP-30 AMPEROMETRIC DETERMINATION OF HYDRAZINE AT NICKEL HEXACYANOFERRATE NANOPARTICLES MODIFIED ELECTRODE**

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**CP-31 SPECTROPHOTOMETRIC DETERMINATION OF MOLYBDENUM-99**

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**CP-32 APPLICATION OF ION CHROMATOGRAPHIC TECHNIQUE FOR THE DETERMINATION OF CHLORIDE IN SERPENTINE**

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**CP-33 ANALYSIS OF NITROGEN BY ICP-AES**

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**CP-34 SEPARATION BEHAVIOUR OF La, Ce, Gd, Dy, Eu AND Sm ON MIXED ION EXCHANGE SURFACE USING MIXTURE OF OXALIC ACID AND DIGLYCOLIC ACID**

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**CP-35 INSTALLATION, COMMISSIONING AND PERFORMANCE EVALUATION OF AN OPTICAL FIBER BASED UV-VIS SPECTROPHOTOMETER**

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**CP-36 CHEMICAL CHARACTERIZATION OF PFBR MOX FUEL**

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**CP-37 A COMPARATIVE STUDY ON DISSOLUTION KINETICS OF SINTERED (Th-U)O<sub>2</sub> PELLETS IN NITRIC ACID BY MICROWAVE AND CONVENTIONAL HEATING**

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**CP-38 STUDY OF THERMAL DECOMPOSITION OF THORIUM OXALATE HEXAHYDRATE**

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**CP-39 STUDIES ON THE THERMAL DECOMPOSITION CESIUM URANYL NITRATE**

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**CP-40 STRUCTURE, MICROSTRUCTURE AND LUMINESCENT PROPERTIES OF RARE EARTH PHOSPHORS FOR WLED APPLICATION**

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**CP-41 DETERMINATION OF ORGANOPHOSPHOROUS CARRIER IMPREGNATED IN SLM**

**Poonam Jagasia, S. Panja, P.S. Dhama, S.C. Tripathi, S.K. Munshi and P.K. Dey**

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**CP-42 ESTIMATION OF Th IN PROCESS SAMPLES IN PRESENCE OF Pu**

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**CP-43 FEASIBILITY STUDIES USING GAS LIQUID CHROMATOGRAPHY AND ION CHROMATOGRAPHY OR THE DETERMINATION OF INDIGENOUSLY SYNTHESISED KSM-17.**

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**CP-44 EFFECT OF DISSOLVED TBP ON THE FLUORESCENCE OF URANYL ION IN NITRIC ACID MEDIUM**

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**CP-45 SPECTROPHOTOMETRIC DETERMINATION OF URANIUM IN OXALATE MEDIUM USING LIQUID WAVEGUIDE CAPILLARY CELL**

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**CP-46 USE OF SIMULTANEOUS SOLID STATE DETECTOR IN INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY(ICP-OES) FOR MULTI-ELEMENT DETERMINATION IN SOIL, SEDIMENTS AND ROCK**

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**CP-47 CHEMICAL & THERMAL CHARACTERIZATION OF SERPENTINE GROUP MINERALS**

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**CP-48 Thermal decomposition studies of sonicated metal oxide-ammonium perchlorate mixtures**

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**CP-49 IDENTIFICATION OF COMPOUNDS PRESENT IN COMPLEX MATRIX BY GCMS USING LRI TECHNIQUE**

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**CP-50 TO STUDY THE EFFECT OF CONDITIONERS ON HAIR BY FTIR WITH ATR ACCESSORY**

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**CP-51 SCREENING OF ACIDIC AND CHELATING EXTRACTANTS FOR THE SOLVENT EXTRACTION OF MIXTURE OF HEAVY RARE EARTHS FROM PHOSPHORIC ACID MEDIUM**

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**CP-52 HPTLC AND LC-MS/MS ANALYSIS OF METHANOLIC LEAF EXTRACTS OF *GLYCOSMISMAURITIANA* (LAMK.) TANAKA**

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**CP-53**

**DETERMINATION OF IRIIDIUM CONTENT IN IRIIDIUM - ALUMINA CATALYST FOR SPACE APPLICATIONS**

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**CP-54 CARBOXYLIC FUNCTIONALIZED WATER SOLUBLE  $\pi$ -CONJUGATED POLYMER: HIGHLY SELECTIVE AND EFFICIENT CHEMOSENSOR FOR MERCURY(II) IONS**

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**CP-55 BIOANALYSIS: AN IMPORTANT STEP IN BA/BE STUDIES**

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**CP-56 DEPTH PROFILE ANALYSIS OF Ni-Fe THIN FILMS USING GLOW DISCHARGE OPTICAL EMISSION SPECTROSCOPY (GD-OES)**

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**CP-57 METHOD DEVELOPMENT FOR THE CHEMICAL CHARACTERIZATION OF NiMnIn, A MAGNRTO-CALORIFIC EFFECT MATERIAL**

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**CP-58 SELECTIVE EXTRACTION AND ESTIMATION OF CALCIUM IN ALUMINIUM FOAM USING EDTA**

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**CP-59 EVALUATION OF MERCURY EXPOSURE USING HUMAN HAIR AS INDICATOR**

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**CP-60 SPECTROMETRIC DETERMINATION OF MALATHION IN DIFFERENT AQUATIC ENVIRONMENTS**

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**CP-61 IMPORTANCE OF IMPURITY PROFILING IN DRUG SUBSTANCES FOR ANALYTICAL METHOD DEVELOPMENT**

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**CP-62 ADVANCED HIGH THROUGHPUT LASER DESORPTION IMAGING TECHNIQUES (LDI)- AN EMERGING ANALYTICAL TOOL IN PROTEOMICS RESEARCH**

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**SP-1 NEXT GENERATION MULTIVARIATE DATA ANALYSIS FOR SPECTRAL DATA**

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## ABSTRACTS/PAPERS

### IT-1

### ICP-MS, RECENT TECHNOLOGICAL ADVANCES, APPLICATIONS AND FUTURE

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The increased application of chemical characterization in several branches of science, such as, material science, metallurgy, geochemistry, mineral exploration, environmental monitoring, semiconductor and nuclear industry is a result of quite some remarkable advances in the area of analytical instrumentation (Balaram, 1996). During the last 25 years, ICP-MS has become a comprehensive analytical technique which revolutionized elemental analyses and has been widely accepted as a powerful tool for trace and ultra-trace elemental and isotopic analysis of most elements, from lithium through uranium, in a variety of materials. The sample preparation methods and analytical instrumentation have steadily and rapidly improved over the last half a century towards achieving lower detection levels for several elements in the periodic table using very small volumes of samples. Analytical chemists can now choose between varieties of instrumental analytical techniques suitable for various applications. When ICP-MS instruments first became commercially available in 1983, they bridged the performance gap between simultaneous elemental measurement and low detection limits. Developments during the last ~ 30 years focused on dealing with matrix issues, specifically polyatomic interferences and on improvements in detection power (Parijat Roy et al, 2007 , Devleena Mani et al 2007). Magnetic sector mass analyzers have been used to resolve some of the isobaric interferences which are impossible to resolve using quadrupole mass analyzers. The magnetic sector instruments are now offering detection limits in parts per quadrillion range (ppq) for several elements. ICP is also coupled to Time of Flight (TOF) mass analyzers with limited success. Recent technological advances in Cool Plasma Technology have helped to eliminate or reduce interferences caused by the argon plasma thus allowing lower detection levels for interference-prone elements such as Li, Na, K, Ca and Fe. The development of Collision/Reaction Cell/Interface Technologies for interference removal in quadrupole instruments has led to some spectacular results in further enhancing the power of ICP-MS (Koti Reddy et al. 2008).

The ability to measure trace element distribution on a micro-scale (spatially-resolved analysis) directly on solids is often critical to our understanding of certain large scale geological processes in geochemical studies. These developments have contributed immensely to the progress of geochemistry, isotopic studies and mineral exploration, especially, for the exploration and mining of uranium, thorium, gold, platinum group elements (PGE) and diamond over the last two decades. Techniques such as LA-ICP-MS (both Quadrupole and Magnetic Sector) have permitted direct simultaneous in-situ elemental and isotopic analysis of solid samples. These techniques are extremely valuable in age dating and mineral exploration studies (Balaram, 2009). Fluid inclusion studies are helpful in understanding aspects, such as, the past history of sedimentary

basins. Hydro-geochemical prospecting methods using ICP-MS are found to be valuable in gold and PGE exploration studies (Balaram, 2008). Coupling ICP-MS with various liquid chromatographic techniques has enabled a unique capability to carry out speciation analysis at ppb levels. The occurrence of arsenic in natural water has received significant attention during recent years (Chandrasekhar, et al.2006). Recent advances in ICP-MS for speciation analysis has helped us to understand the toxicity and bioavailability of arsenic in different compartments of our environment. Therefore, it is likely that these advances in analytical instruments, especially in ICP-MS will have a greater impact on future studies in different branches of Science and Technology. Lot of research and development studies are going on at present in different laboratories world over for further improvements in ICP-MS technology.

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## IT-2.

### NEW ORGANIC FUNCTIONAL MOLECULES FOR CHEMO/BIO SENSORS

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In this presentation, I will first describe some new tetrathiafulvalene (TTF) molecules for chemical sensors, by making use of the unique feature of TTF (and its derivatives), which can be reversibly transformed into the radical cation  $TTF^{\bullet+}$  and dication  $TTF^{2+}$  through either chemical or electrochemical oxidations at easily accessible potentials. These include chemical sensors towards  $^1O_2$ ,  $Hg^{2+}$ , saccharides based on TTF-anthracene dyads.<sup>1-5</sup> In addition, I will introduce new chemo-/biosensors including DNA detection method and label-free fluorescence nuclease assay based on the aggregation-induced enhanced emission (AIE) of silole.<sup>6-12</sup>

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### IT-3

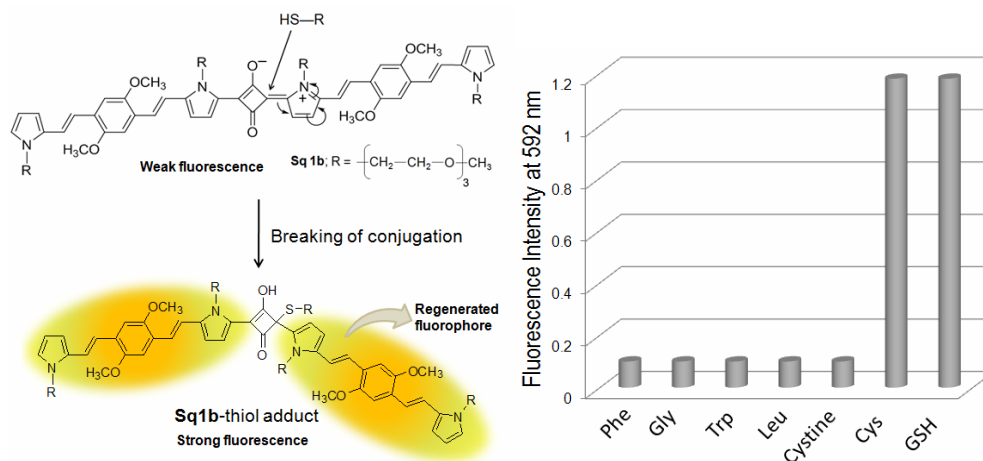
#### RATIONAL DESIGN OF MOLECULAR PROBES FOR BIOLOGICALLY RELEVANT ANALYTES

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Selective detection of a specific analyte in the presence of other competing species is a challenging problem in analytical chemistry. A large number of molecular probes have been reported in recent years for this purpose. In such cases, the analyte binding is signaled with the change in one of the properties such as absorption, emission or redox behavior, arising out of electron transfer, charge transfer, excimer formation or conformational changes. Among different methods, fluorescence technique is preferred due to the high sensitivity of the signal. We have been interested in developing fluorophores, useful for the selective detection of biologically important cations and neutral molecules. With this objective, recently we have exploited squaraine dyes, a class of organic dyes for the design of molecular sensors.<sup>1-3</sup> Subsequently, we have reported a novel strategy for the detection of total aminothiols content in human blood plasma using a near infrared absorbing squaraine dye which is sensitive to thiol attack. Details of these studies will be discussed.



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## IT-4

### TUNING OF EMISSION COLORS WITH LANTHANIDE COMPLEXES: FACILE PHOTOLUMINESCENT PRODUCTION OF TRUE WHITE LIGHT

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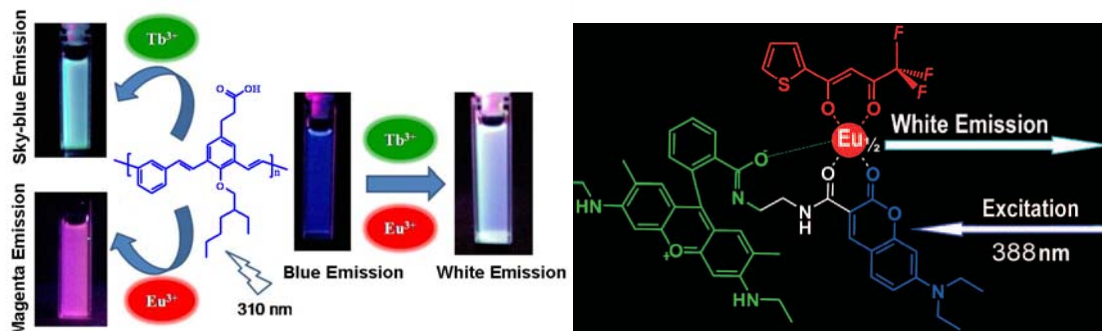
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White organic light-emitting diodes have been of considerable interest in recent years due to their potential applications as full color displays, backlights for liquid crystal displays and solid-state lighting sources [1]. Thus, white emission should ideally be composed of primary colors (red, blue and green) or complementary (i.e. blue and yellow or orange) colors and cover the whole visible range from 400 to 700 nm, and the emitter should have the ability to emit the primary colors simultaneously with equal intensities to produce white light and the pure colors separately in a tunable way [2]. Traditional methods of such weight light generation typically rely on mixing the various primary colors from different emitting materials [3]. An alternative approach for the generation of efficient white light is to use a single-component emitter, which can have advantages such as greater stability, better reproducibility, no phase separation and simpler fabrication processes [4]. Although a few materials show white-light emission as single component, none has been reported to produce well separated blue, green and red emissions besides white light. Since the energy transfer typically quenches one or

more of the emission pathways and thereby restricts the transitions that define the output spectrum, the design of color tunable single-component emitters requires readily tailorable different fluorophores and fine-tuning of the energy transfer processes between different fluorophores. On the other hand, lanthanide containing materials, which exhibit excellent sharp-emissions luminescence properties with suitable sensitization, have attracted considerable interest and been effectively used in designing of white-light nanoparticles [5]. With judiciously chosen red- ( $\text{Eu}^{3+}$ ,  $\text{Pr}^{3+}$ ,  $\text{Sm}^{3+}$ ), green- ( $\text{Tb}^{3+}$ ,  $\text{Er}^{3+}$ ) and blue-emissive ( $\text{Tm}^{3+}$ ,  $\text{Pr}^{3+}$ ,  $\text{Ce}^{3+}$ ,  $\text{Dy}^{3+}$ ) ions doped in a suitable host, it is possible to obtain phosphors which emit across the entire visible spectrum with high color purity [6,7]. Here, we review some of the seminal work in the area, along with new developments in the field. From our laboratory, we have demonstrated a facile molecular approach to generate white light emission by combining carboxylic functionalized poly(m-phenylenevinylene)s polymeric architectures with lanthanide  $\beta$ -diketonate complexes [8]. Investigations revealed that carboxylic functionalized polymeric material with  $\text{Eu}^{3+}$ - $\beta$ -diketonate complex exhibits unique magenta emission when excited at 310 nm. On the other hand, carboxylic functionalized polymeric material with  $\text{Tb}^{3+}$ - $\beta$ -diketonate complex shows bright sky-blue emission. Interestingly, when  $\text{Eu}^{3+}$  and  $\text{Tb}^{3+}$  were incorporated into polymer backbone in equimolar ratio along with acetyl acetone as co-ligand, exhibited a white emission with CIE 1976 color coordinates  $x = 0.28$ ,  $y = 0.34$ .

Recently, a new fluorophore that exhibits tunable emission of three primary colors and white light, by combining an  $\text{Eu}^{3+}$  moiety as the origin of red light with an organic ligand that comprises a blue-emitting coumarin fluorophore and a green-emitting Rhodamine G fluorophore [9].



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## IT-5

### HPTLC IN FOOD ANALYSIS: SPECIAL EMPHASIS ON ANALYSIS OF FOOD ADDITIVES,CONTAMINANTS AND MYCOTOXINS

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Chromatography is one of the oldest and widely used techniques as a method of separation of components in a mixture by a variety of phenomena such as partition, adsorption, ion exchange etc.

The Russian botanist Tswett discovered adsorption chromatography, but this passed unnoticed until 1931. He observed that plant pigments like chlorophylls could be separated by filtering their solution in petroleum ether using a column containing calcium carbonate. It was noticed that yellow and green zones were formed on the column. He remarked that "like rays of light in a spectrum, the various components of a mixture of pigments are separated in a definite order and can then be determined qualitatively and quantitatively". He separated leaf extracts into coloured bands using an inulin column. Separation of coloured oils when percolated through earth was observed by Day<sup>3</sup>. However, the former is usually credited, by and large, with the discovery and description of chromatography. The term "chromatography" literally means "description of colours" was suggested, because first separations involved, of necessity, coloured components.

Chromatography has been one of the oldest and being widely used techniques, as a method of separation of components in a mixture. Thin layer chromatography known as planer chromatography was earlier a stagnant technique. But due to advancement in instrumental techniques and development in hyphenated techniques, High performance thin layer chromatography became one of the important tools capable of giving fast results, high resolution, and separation of more accurate and precise quantitative results with many advantages over other techniques. Thin layer chromatography is widely used for food analysis and quality assessment throughout the world. Literature reveals numerous applications in the domain of food composition, for verification of food labeling, additives, adulterants, contaminants, decomposition related to determinations of compound classes such as amino acids (protein for determination of quality), lipid and fatty acids (for evaluating quality and adulteration in oils/fats), sugar (beverages), androgenic amino acids (for assessing storage stability), vitamins, nutrients, colorants, antioxidants, preservatives, special quality factors and carbohydrates.

Various separation techniques like HPTLC, HPLC and GC have their own advantage and disadvantage. A general comparison is given below.

#### Comparison of HPTLC, HPLC, and GC

S. No	HPTLC	HPLC	GC
1	Small amount of mobile phase required.	Large amount of mobile phase required.	Large amount of mobile phase required.
2	Temperature & Pressure control not required.	Temperature & Pressure control required.	Temperature & Pressure control required.
3	Off line system	On line system	On line system
4	One can visualize the sample.	One cannot visualize the sample.	One cannot visualize the sample.
5	It's a multiple sample process.	At a time only one sample can be processed.	At a time only one sample can be processed.
6	Economical	Expensive	Expensive
7	Sample preparation is minimal.	Sample preparation is tedious.	Sample preparation is tedious.
8	It's the fastest technique.	Comparatively slow.	Comparatively slow.
9	Low maintenance	High maintenance	High maintenance

Food additive means any substance not normally consumed as a food by itself or used as a typical ingredient of the food, whether or not it has nutritive value, the intentional addition of which to food for a technological (including organoleptic) purpose in the manufacture, processing, preparation, treatment, packing, packaging, transport or holding of such food results, or may be reasonably expected to result (directly or indirectly), in it or its by-products becoming a component of or otherwise affecting the characteristics of such food but does not include "contaminants" or substances added to food for maintaining or improving nutritional qualities;

Contaminant means any substance, whether or not added to food, but which is present in such food as a result of the production (including operations carried out in crop husbandry, animal husbandry or veterinary medicine), manufacture, processing, preparation, treatment, packing, packaging, transport or holding of such food or as a result of environmental contamination and does not include insect fragments, rodent hairs and other extraneous matter;

Contaminants in food refer to undesirable materials present in small quantity/traces, which are incorporated in food inadvertently or due to negligent handling, processing, storage, transportation etc. in the food chain. These toxics may be injurious to health at a low level and thus constitute a part of food safety quality assurance system. Due to liberalization of world market, maximum permissible limits of these contaminants play an important role in marketing of food from one country to

another country or even within the country. National and International directives are very stringent in these regards.

Mycotoxins are secondary metabolites of moulds. The most important mycotoxins are Aflatoxins, Deoxynivalenol, Ochratoxin A, Fumonisin, Patulin, Zearalenone and T-2 toxins. These may contaminate crop plants, fruits, nuts, and grains before or after harvest. The toxic impacts of mycotoxins on human and animal health are proven beyond doubt.

Application of HPTLC for detection/determination of Aflatoxin, mycotoxins vital contaminants in foods at the lowest level is an inspiration for use of this instrument, as an official/validated method for determining and screening.

HPTLC is an effective, cheaper and simple quantitative method undertaken on layers composed of smaller particle size i.e., 5  $\mu\text{m}$  approx. as compared to 12-25  $\mu\text{m}$  for TLC. Distribution of particle size is necessary, with thinner layers and development distance is shorter for HPTLC, thus leading to greater and quick separation effectively with better detection limits. HPTLC has several advantages over the other instrumental techniques being used in the field of food analysis. Specially modified and with more advancement of HPTLC coupled with AMD system etc. has proved to be boon in evaluating contaminants at a much lower level with a better reproducibility of results. In India, assessment of quality of food is a biggest challenge.

#### **GENERAL APPLICATIONS**

Carbohydrates, Organic Acids, Food grains, Lipids, Fats & Oil, Protein and Amino Acids, Food contaminants/Additives/ Colours/Adulterants etc, Pesticide Residues, Mycotoxins, Antibiotics and Drugs Residues in Food, Pigments and Dyes, Essences, Wines, Fruits & Vegetables, Spices & Essential Oils, Alkaloids, Vitamins

#### **SPECIFIC APPLICATIONS**

Detection of Anti-oxidants in edible oil, Quantification of Caffeine in tea, Quantification of Caffeine in coffee, Identification of Cholesterol in edible oil, Quantification of Nicotine in tobacco, Finger print of Saffron, Detection of Castor oil in edible oils, Determination of eugenol in clove oil, Quantification of piperine in Piper Nigrum, Detection of formaldehyde in milk, Identification of chicory in coffee, Identification of Preservatives in tomato sauce, Quantitative Determination of Gingerol in Ginger, Detection of Argemone in edible oil, Quantitative Determination of Aflatoxin  $M_1$  in Milk & Milk Products, Determination of Aflatoxin  $B_1, B_2, G_1$ , and  $G_2$  in foodstuffs, Quantitative Determination of Sucralose in Indian Sweets (burfi), Separation of Sugars, Quantitative Determination of Pesticides residues in Grapes, Determination of Cylopiazonic acid in foodstuffs, Determination of mono-, Di-, Tri- and Polysaccharides in food stuffs, Quantitative Determination of Vitamin C in fruit juice, Determination of lactose, saccharose and fructose/ glucose, Identification and Determination of p-hydroxybenzoic acid, its esters and 4-methoxycinnamic acid derivatives, Quantitative Determination of Salicylic acid and its derivatives, Quantitative Determination of

Cholesterol in fat emulsions with AMD, Determination of rapeseed oil in fermentation broth, Quantitative determination of amino acids in potatoes, Determination of pesticides in drinking water, Determination of Phospholipids in foods, Identification and Quantitative Determination of Sugars in Beer and Wine, Analysis of Quinolonic Antibiotics in Fish and Fish Feed, Quantitation of Glycerol in Tobacco,

Determination of Sucralose and Fructose in Food and Beverages, Determination of Organic Acids in Wine, Quantitative Determination of Vitamin D<sub>3</sub>, Analysis of Oligosaccharides in Molasses, Analysis of Inorganic and Organic Mercury in Water, Simultaneous quantitative determination of Vitamin D analogs (provitamin D, irradiation products of provitamin D, vitamins D<sub>2</sub>-D<sub>3</sub>, vitamin D esters), Detection and Semi quantitative determination of anabolica in meat, Analysis of Curcuma Longa for curcumin, Determination of Glycin, Alanine and Leucine Amino acids in Fish scales, Detection of Arabinose and Xylose in Gums, Separation of Ergot alkaloids, Quantification of Pesticides in Egg Powder, Determination of Selenium in water , Detection of Mineral Oil in Edible Oils, Detection of Tricresyl Phosphates in Edible Oils Etc.

### **Conclusions**

HPTLC is a versatile technique with wide application in food ,drug, cosmetics, herbal etc. The technique is simple, cheaper , convenient and suitable for screening large number of samples at a time.

### **IT-6**

#### **ELECTRON MICROSCOPY: AN INEVITABLE TOOL FOR MATERIALS CHARACTERIZATION**

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Electron Microscopes are widely used as an indispensable tool for research and development and have a central role to play in many fields such as pathology, environmental science, forensic science, industrial development, molecular biology, genetic engineering and many other high technology fields concerned with semiconductors and other new materials. The contribution of electron microscopy to materials science has led to the development of new materials ranging from light weight, high strength alloys for space applications to heavy weight alloys like lead shielding, uranium and zirconium alloys for nuclear reactors, corrosion resistant (Cr-Mo) soft austenitic stainless steel, hard and brittle, martensitic stainless steel, super alloys (Ni or Co) and super plastic alloys etc.

Electron microscopy has demonstrably had a significant positive impact on our society as materials are increasingly tailor-made on an atomic scale to meet the specific needs. With the advent of new technology and improvement in electron microscopy, new discoveries on the structure property relationships of materials become possible at ever decreasing scales. Electron microscopy and micro chemical analysis will make a greater and central contribution in the microstructure characterization of organic & inorganic materials. Electron microscopy has become the science of understanding the microstructure properties and subsequent characterization of materials. Characterization of materials by electron microscopic techniques is very important in the field of current research in materials science. The informations such as surface morphology, topography, composition and crystallographic details etc can be yield from the SEM, TEM images of materials which in turn help to understand the basic properties like conductivity, electrical properties, strength etc of them.

Macroscopic behavior of materials is dependent on the elemental compositions at micro scale. Energy Dispersive X-ray Spectrometer (EDS) is an analytical tool which is used in conjunction with Electron microscope for the elemental analysis of materials in micro range. Its characterization capability is supported on the fundamental principle that interaction of the primary beam of electrons with atoms in the sample causes shell transition which may result in the emission of X-ray which is the energy characterization of the parent element. Thus EDS can endow with rapid qualitative, quantitative analysis of the elemental composition with sampling depth of 1-2 microns. Elemental constituents can be determined to the concentration ranging as low as 100ppm thus allows us to determine and measure the minutest trace of constituent elements. Electron Microscopy and Energy Dispersive Spectroscopy are the keywords for novel and ground-breaking studies in the multidisciplinary areas of material research in chemistry, biochemistry, environmental and energy science, material science and medical science. The main intention of the keynote address is to provide vital know-how of the ground rules for getting the best microstructure and to bring in the concepts of the most efficient and robust approach to analyze materials, Energy Dispersive Spectroscopy.

#### IT-7

### **ANALYSIS AND ENVIRONMENTAL LOADING OF PHARMACEUTICAL AND PERSONAL CARE PRODUCTS FROM HEALTHCARE FACILITY WASTEWATER USING SELECTIVE ION EXTRACTION AND UPLC - TANDEM MASS SPECTROSCOPY**

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Presence of Pharmaceuticals and Personal Care Products in the wastewater effluents and potable supplied water has increased the need to develop a method to identify these emerging contaminants at their sources. A rapid selective solid phase extraction followed by ultra performance liquid chromatography in combination with triple quadrupole mass spectrometric (UPLC - MS/MS) method was used for detection of 48 pharmaceuticals and 6 metabolites in the healthcare facilities wastewater. Fifty four pharmaceuticals were distributed across 9 of the 14 therapeutic categories from Anatomical Therapeutic Chemical (ATC) classification system. Pharmaceuticals included were 4 from ATC Code A (alimentary tract and metabolism), 1 from ATC Code B (blood and blood forming organs); 18 from ATC Code C (cardiovascular system), 3 from ATC Code G (genito-urinary system and sex hormones), 5 from ATC Code H (systemic hormonal preparations, excluding sex hormones and insulin), 2 from ATC Code J (anti-infectives for systemic use), 2 from ATC Code M (Musculo-skeletal system), 14 from ATC Code N (Nervous system) and 5 from ATC Code R (respiratory system). Oasis MCX, mixed mode reverse-phase / cation-exchange cartridge, was used for single cartridge extraction for all the analytes. Due to the complexity of the sample matrix, the acceptable target matrix spike recoveries were set between 60% and 140%. All analytes were quantified with single extraction and four chromatographic runs with the method detection limit for different analytes ranging from 1 to 51 ng/L. Wastewaters from four

independent healthcare facilities from the same municipality sewer system were analyzed. Forty-one out of the 54 analyzed pharmaceuticals were detected in at least one facility's wastewater, with 21 of the total analytes found in wastewater from every facility. The maximum mean analyte concentration within each ATC code was 0.9 µg/L ranitidine for ATC code A; 0.07 µg/L warfarin for ATC code B; 14.6 µg/L valsartan for ATC code C; 0.4 µg/L hydrocortisone for ATC code H; 178 µg/L sulfamethoxazole for ATC code J; 30 µg/L ibuprofen for ATC code M; 0.3 µg/L amitriptyline for ATC code N; and 0.2 µg/L hydrocodone for ATC code R. Each facility's daily wastewater flow was combined with individual analyte concentrations to estimate the mass loading of pharmaceuticals leaving each facility through wastewater discharges to the municipal sewer system on the sampling date. The total estimated daily mass loading of all measured pharmaceuticals ranged from 1 g/day at the assisted living facility to 31 g/day at the hospital. The combined loading for all four facilities was 58 g/day. These findings provide a basis for future research needed for risk management of pharmaceutical sources to the environment.

#### IT-8

### RECENT INVESTIGATIONS IN AAS : MATRIX EFFECTS IN GFAAS and DEVELOPMENT OF ICP-AAS

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Atomic emission spectrometric (AES) and atomic absorption spectrometric (AAS) methods are found suitable for determination of trace elements, in nuclear materials. However, AES based methods are preferred because of their capability to determine a large number of elements simultaneously. The analytical methods based on AAS have found a role in nuclear fuel analysis for providing independent check. There are a few reports based on use of AAS methods after chemical separation of major matrices. In our laboratory we have developed methods for the determination of a number of elements directly using GF-AAS technique which has the capability to determine many of these elements at sub-ppb levels. Two major problem encountered in GF-AAS technique are (i) severe suppression in the absorbance for the majority of analytes in the presence of U/Pu/Th/Zr matrices in comparison to simple aqueous solutions and (ii) the technique is not suitable for refractory and carbide forming elements. In our laboratory efforts have been directed to understanding these matrix effects and developing an AAS unit using ICP as atomizer (ICP-AAS) so that it will enable atomization of refractory elements. For understanding matrix effects in GF-AAS, studies were carried out to identify the changes in surface morphology, and the elements and compounds formed on surface using SEM, EDAX and XRD technique in addition to GF-AAS measurements such as changes in absorption characteristics (peak height and absorption profile), appearance temperature and activation energies in presence of U/Th/Zr/ Aqueous matrices. In the case of ICP-AAS, since commercial units are not available, such a unit was designed and assembled in-house. The salient features of these investigations will be discussed.

## IT-9

### THE ROLE OF MODERN ANALYTICAL APPROACHES IN TEMPLATE ASSISTED CONDUCTING POLYMER NANOMATERIALS

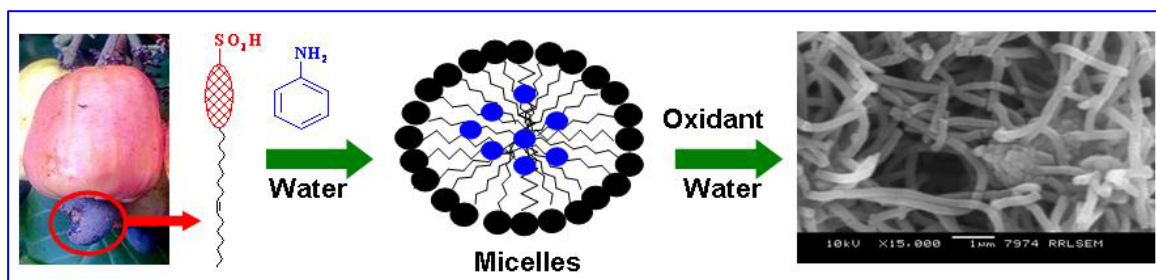
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Conducting nano-materials have attained wide interest due to their unique electrochemical properties and processability in electronic and optical devices such as energy storage devices, opto-electronics, chemical sensors, biological sensors, actuators etc. Understanding the mechanism of the formation of these new classes of organic based electronic nanomaterials is emerging as very important task for reproducible research as well as sustainable to long term technological developments. We have recently developed unique and novel self-assembled molecular approaches to selectively template polyaniline and polypyrrole nano-materials. Self-assembly of custom designed amphiphilic molecules produced cylindrical, spherical, vesicular and supramolecular organogel nanotubular templates which were polymerized in emulsion, dispersion and interfacial routes to fabricate various conducting nanomaterials. Various nanostructures such as nano-fibers, nano-rods, nano-spheres and nano-tubes, etc were obtained by precisely controlling the molecular templates. During the course of development of these nanomaterials, we put significant effort to understand the molecular interaction in the templates. Modern analytical spectroscopic tools such as dynamic light scattering, high resolution electron microscopes, NMR, FT-IR and Wide angle X-ray diffractions were utilized to trace the mechanistic aspects of these template-assisted synthetic process. Further, the synthesized nanomaterials were also employed as sensor for chemical and biological substances. The presentation will be focused on the recent developments in our research group in the above topic and will also demonstrate the need for the systematic analytical approaches for sustainable nanomaterials research.



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IT-10

## ICP-AES AS APPLIED TO METALLURGICAL INDUSTRY

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Inductively Coupled argon Plasma Atomically Emission Spectrometry(ICP-AES) as an analytical technique is known for its uniformly good sensitivity both for volatile and refractory elements, large linear dynamic range and relatively good freedom from chemical and ionization interferences. Thus it scores over many other competing techniques in its varied application areas.

Metallurgical industry needs determination of trace, minor and major constituents of various types of alloys apart from determination of few isolated elements at sub ppm levels. At times, some process-intermediates and process contaminants also need to be monitored. In this regard, ICP-AES provides a good helping hand to the industry in its quest for quality products. With the better precision feasible with the technique, it scores over spark based optical emission spectrometry. Metallurgical industry, both for ferrous and non ferrous alloys, is blessed with the availability of varied types of internationally accepted, certified reference materials. These are fruitfully utilized singly or in combination with two or three in preparing the working standards. A calibration curve generated from aspiration of these standards then serves to provide analysis of a given sample. A certified reference material other than the ones used in the preparation of working standards can be used as a control sample or check sample prior to analysis of real samples to make sure the correctness of calibration procedure. Thus, validation of analytical data is automatically achieved.

A computerized ICP Spectrometer with Echelle grating optics, a good sized and modified version of CCD with peltier cooling and a RF generator feeding power to a Mini-Torch serves as the experimental facility.

The procedure adopted as above holds good for a wide range of concentrations of constituent elements. These concentrations also include percentage level determination. By choosing a semi-micro-balance(0.01 mg readability) small sample size is chosen and on dissolution, the sample solution volume is made up to 50-100 ml. With reasonably small sample size and large final volume, one actually determines only microgram/ml amounts of analytes which runs reasonably well with the basic aim of using ICP-AES technique

Further, barring the detector saturation(a rare phenomenon for normal concentrations with charge couple devices(CCD)) signal saturation can be tackled with alternative analytical spectral lines. Matrix effect if any, is taken care of by including matrix blank as the first standard in the calibration programme.. Such a procedure has helped optimization of a number of analytical methods for the analysis of variety of

alloy samples in the laboratory having accreditation with NABL, ISO and other certifying agencies.

The methods developed and used for day-to-day analysis include those for compositional characterization of various types of steels, copper base alloys, etc. The data obtained from the analysis of some of these matrices will be presented to establish utility of such an approach to establish utility of such an approach in ICP-AES.

## IT-11

### HYPHENATED TECHNIQUES: LC-MS

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Chromatography is a versatile technique for separation of all types of compounds in its different forms: namely: GC, HPLC, IC, HPTLC etc. It has a great separation capability and achieves very low detection limits with the use of very sensitive detectors. It's only draw back is, it does not provide qualitative confirmation about the compounds separated and identification or structural elucidation of the compounds.

Spectroscopy is another branch of analytical chemistry, which gives information about the structure of organic compounds with the techniques involving UV-Visible Spectroscopy, FTIR, and NMR etc. The combination of Chromatography with Spectroscopy can provide structural information on the compounds of interest.

Mass Spectrometry (MS) is the technique which can give the information on structural elucidation of the organic compounds by fragmenting the molecule and measuring the intensity of the fragment ions against  $m/z$  (mass to charge ratio of the fragmented ion). The spectrum is like a fingerprint.

The combination of these two great analytical tools (Chromatography-Spectroscopy) is what Hyphenated Technique means.

The GC-MS and LC-MS have shown the versatility in terms of sensitivity, selectivity, structural elucidation etc and have become more popular in the R & D and also for Quality Control. The application areas are growing rapidly and cover a very wide spectrum. The talk covers High performance Liquid Chromatography (HPLC), or also referred as just LC (Liquid Chromatography), hyphenated to Mass Spectrometry, The LC-MS.

LC-MS is one of the most popular and recently developed Hyphenated techniques, which has rapid growth in last decade and majority of the applications are in pharmaceutical and biotechnology field.

In this lecture the following aspects are covered:

- The History of development of LC-MS especially in developing interface between LC and MS
- The current Interface technologies: Atmospheric Pressure Ionization (API)
- Mass Spectrometers used in LC-MS applications
- The concept of Tandem Mass Spectrometry
- The Use of Triple Quadrupole Mass Spectrometer, Tandem MS (LC-MS/MS)
- Hybrid Tandem Mass Spectrometry with LC and its applications.
- The Applications of LC-MS in Pharmaceutical and biotechnology fields.

## IT-12

### GAS CHROMATOGRAPHY-MASS SPECTROMETRY (GC/MS): EMERGING VISTAS OF THE APPLICATIONS

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Hyphenation of Chromatography to mass spectrometry has led to identification and characterization of various organic species in different matrices. This allowed, for the first time, the analysis of multicomponent mixtures of analytes without employing cumbersome separation methods. The development of GC-MS was the trigger for the development of modern mass spectrometry. Immense potential of chromatographic separations for resolving multicomponents mixture using capillary column gets synergically coupled to state of the art mass spectrometric detector. Interesting applications of GC-MS include Drug detection, explosives/arson investigation, Environmental analysis, Food technology Forensic science etc. GC-MS can also be used in airport security to detect substances in luggage or on human beings. New ionisation techniques developed over the last 25 years (fast particle desorption, electrospray ionisation and matrix-assisted laser desorption / ionisation) have opened up the world of biological chemistry to mass spectrometry.

The GC-MS has been widely heralded as a "gold standard" for forensic substance identification because it is used to perform a specific test. A specific test positively identifies the actual presence of a particular substance in a given sample. Although a non-specific test could statistically suggest the identity of the substance, this could lead to false positive identification. Real excitement in the application of GC-MS lies in its ability to determine the identity of key components present in criminal/ Forensics particles from a human body that provide important link to a crime. GC-MS is increasingly used for detection of illegal narcotic, and may eventually supplant drug-sniffing dogs. Security: A post-September 11 development is that, explosive detection systems have become a part of all US airports. These systems run on a host of technologies, many of them based on GC-MS.

It is becoming the tool of choice for tracking organic pollutants in the environment. For most organic analysis of environmental samples, including many major classes of pesticides, it is very sensitive and effective. In combination with isotopic labeling of metabolic compounds, the GC-MS is used for determining metabolic activity.

A mass spectrometer is typically utilized in one of two ways: Full Scan or Selective Ion Monitoring (SIM). The typical GC/MS instrument is capable of performing both functions either individually or concomitantly. A "full spectrum" analysis considers all the "peaks" within a spectrum. However, selective ion monitoring (SIM) which looks only at a few characteristic peaks associated with a candidate substance, can also be done. GC-MS has found potential in the quality evaluation of various solvents used for processing of nuclear materials. New ionization techniques like fast particle desorption, electrospray ionisation & matrix-assisted laser desorption) have induced extensive use of mass spectrometry in biomedical field. The inherent characteristics of TOF-MS are extreme sensitivity, unlimited mass range and speed of analysis. This makes TOF-MS one of the most desirable methods of mass analysis.

**GAS CHROMATOGRAPHIC DETERMINATION OF MONOMERS IN THE  
ACRYLIC COPOLYMER EMULSION**

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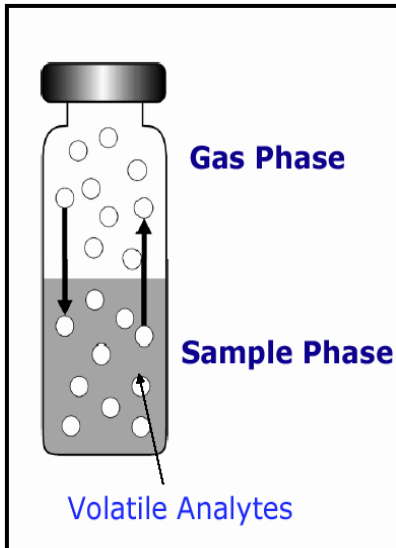
Monomers such as a Styrene, Acrylonitrile and Butyl Acrylate are used to manufacture acrylic co-polymer emulsions. Such copolymers are used to prepare adhesive laminations, fabric coatings, exterior auto paints etc. Excessive amounts of unreacted monomers beyond specific limits in the co-polymer product may cause concerns relating to toxicity and odor. Hence a reliable analytical method is required to monitor and determine the unreacted monomers in the co-polymeric emulsions. Direct syringe injection methods on GCs are reported in the literature, however subsequently problems were observed in such GC method because of thermal degradation of polymeric matrix in the hot injector port. Pyrolyser GC and HPLC methods are also reported in the literature with variable degree of success. A simple and reliable Headspace (HS) - Gas Chromatographic (GC) method is reported in the present work for the determination of monomers such as Acrylonitrile, Butyl acrylate and styrene in acrylic co-polymer emulsion samples. A static head space sampler, coupled with split injector capillary GC (Thermo Fisher Scientific make Chemito-CERES-800 plus model) with FID and PEG Capillary column was used for the said analysis of monomers. The peaks of all the three monomers were clearly resolved, identified and quantified. The retention times (RT) were found at about 4.9, 12.5 and 15.4 minutes for acrylonitrile, butyl acrylate and styrene respectively. Thus the present HS-GC method would be very useful in the routine QA/QC work of the relevant polymer industries.

**INTRODUCTION :**

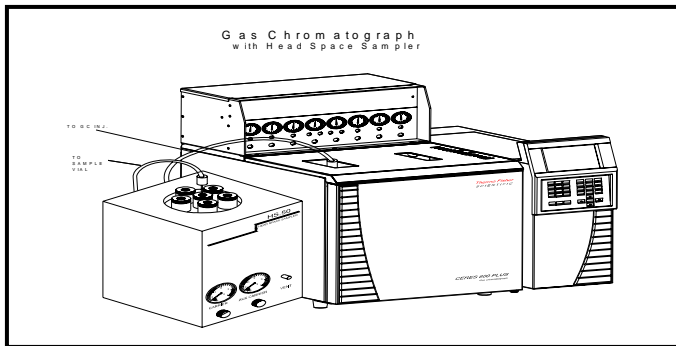
Monomers such as a Styrene, Acrylonitrile and Butyl Acrylate are used to manufacture acrylic co-polymer emulsions. Such copolymers are used to prepare adhesive laminations, fabric coatings, exterior auto paints etc. Excessive amounts of unreacted monomers beyond specific limits in the co-polymer product may cause concerns relating to toxicity and odor. Hence a reliable analytical method is required to monitor and determine the unreacted monomers in the co-polymeric emulsions. Direct syringe injection methods on GCs are reported in the literature, however subsequently problems were observed in such GC method because of thermal degradation of polymeric matrix in the hot injector port (1). This problem was sorted out by extraction of free monomers from polymeric matrix by extractive distillation (2) or by precipitating the polymer with concentrated acids and extraction of free monomers by using water immiscible solvents (3). Pyrolyser GC (4) and HPLC methods (1) are also reported in the literature with variable degree of success. A simple and reliable Headspace (HS) - Gas Chromatographic (GC) method is reported in the present work for the determination of

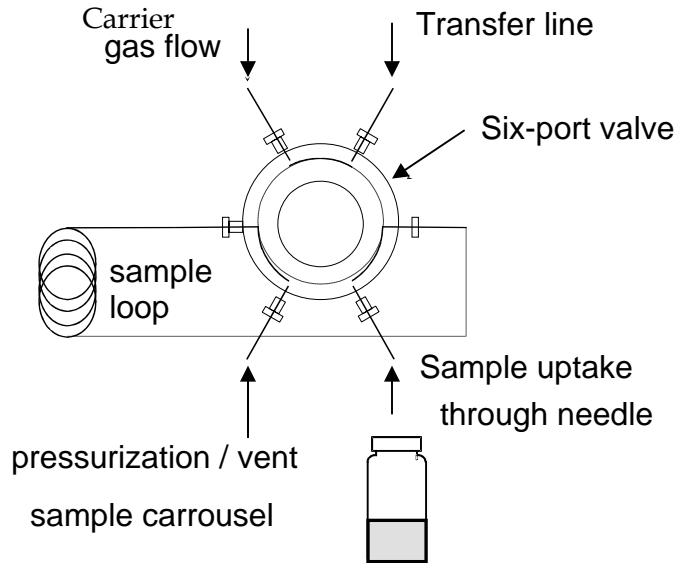
monomers such as Acrylonitrile, Butyl acrylate and styrene in acrylic co-polymer emulsion samples. A static head space sampler, coupled with split injector capillary GC (Thermo Fisher Scientific make Chemito-CERES-800 plus model) with FID and PEG-Capillary column was used for the said analysis of monomers.

**Head Space Sampling ( HSS ) Technique :** A liquid or solid sample is heated in a sealed vial. Equilibrium is established between the sample and the gas phase Headspace). Aliquot of the gas phase is transferred to the GC.



Head Space sampling is a technique of introducing volatile components from a solid or liquid sample into GC when actual sample is difficult to inject because of the nature of sample matrix





### Transfer mechanism of headspace contents to GC

**Gas Chromatographic Analysis:** Among the various analytical techniques available, Gas chromatography (GC) has special significance, as it is a powerful separation technique with high degree of resolution and good sensitivity.

GC equipped with split / split less injector, Capillary column and Flame Ionisation Detector (FID) coupled with static Head Space Sampler (HSS) can be used for the separation, detection and quantitative estimation of such monomer traces / contents in acrylic polymer emulsion.

### EXPERIMENTAL:-

**Chemicals:** - Double distilled/ HPLC grade water, standards of monomers, such as Styrene, butyl acrylate and acrylonitrile were obtained.

**Sample Preparation and Gas Chromatographic Analysis :** 1 ml of HPLC grade Water as a blank, 1 ml of standard solution containing 0.5% each of Styrene, butyl acrylate and acrylonitrile in HPLC grade water and 1 ml of aqueous acrylic co-polymer emulsion samples were separately incubated at 100 degree C for 30 minutes and then introduced through HSS into the GC injector.

Gas Chromatographic (GC) studies were carried out using a Thermo Fisher Scientific, Chemito CERES 800 plus Model of GC ( [www.thermofisher.com](http://www.thermofisher.com) ) having capillary split / split less injection port with a Flame Ionization Detector (FID) and Iris 32 software, was used for data processing. The capillary column used in the present studies was

(Polyethylene Glycol) capillary column having 30 m length, 0.32 mm ID, 1.0  $\mu$ m film thickness.

**GC Analytical Conditions:** The GC analytical conditions were set as follows:

**GC with capillary split/ split less injection port and FID detector,**

**Polyethylene Glycol capillary column** having 30 m length, 0.32 mm ID, 1.0  $\mu$ m film thickness.

Injector : 220°C, Detector: 240°C,

Oven programming conditions:60°C with ramp rate of 4°C/min.to 220°C with 1 minute  
Final hold,

Split ratio: 1:100, sensitivity range : 1,

Auxiliary 1 and 2 temp: 90 ° C (for heating the carousel and the transfer line)

Carrier gas :(Nitrogen )

Flow : 1 ml / min., Sample volume -1.0 ml of HS.

## **RESULTS AND DISCUSSIONS :-**

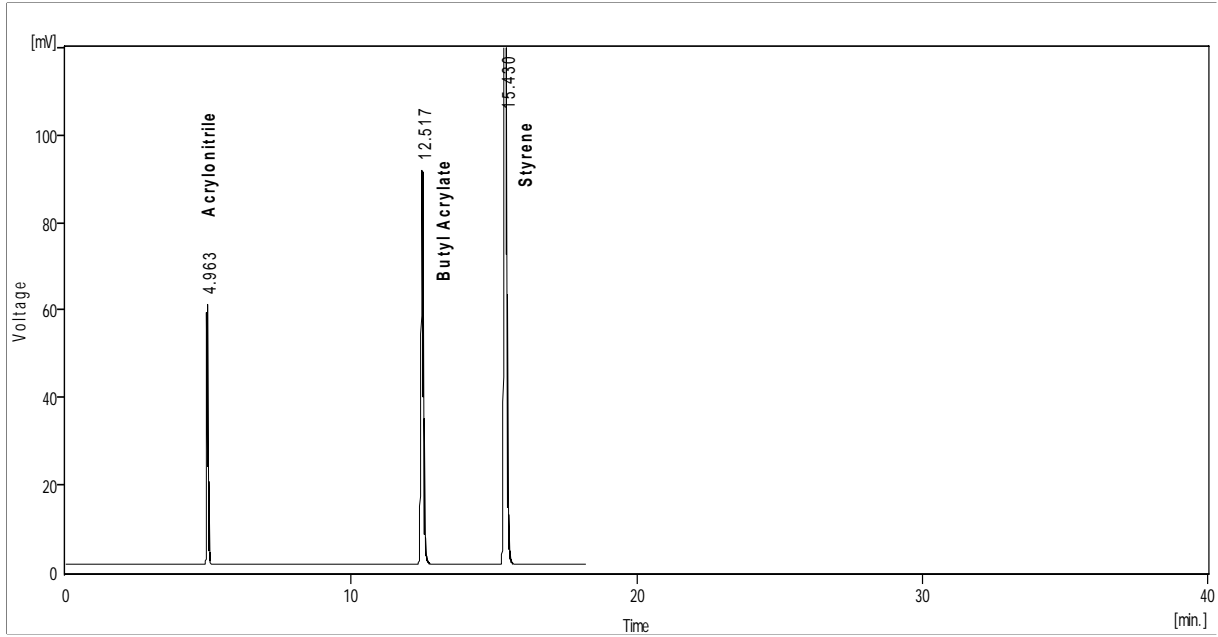
It was first confirmed with GC-HSS analysis of 1 ml of HPLC grade Water that there were no peaks in the chromatogram of the blank. GC-HSS analysis results for 1 ml of standard sample containing 0.5% each of Styrene, butyl acrylate and acrylonitrile in HPLC grade water and that for 1 ml of some typical aqueous acrylic emulsion samples are shown in Fig. Nos. 1, 2 and 3 respectively. Retention Times for Acrylonitrile, Butyl acrylate and styrene were observed at ~ 4.9, 12.5 and 15.4 minutes respectively. These results indicate a clear baseline separation of all the three monomers of interest on PEG Capillary column and that the quantification done by using external standard method was found to be satisfactory. The results of the present work for the monomer content in typical acrylic polymer sample Nos. 1 and 2 are given in Table 1.

## **CONCLUSIONS:-**

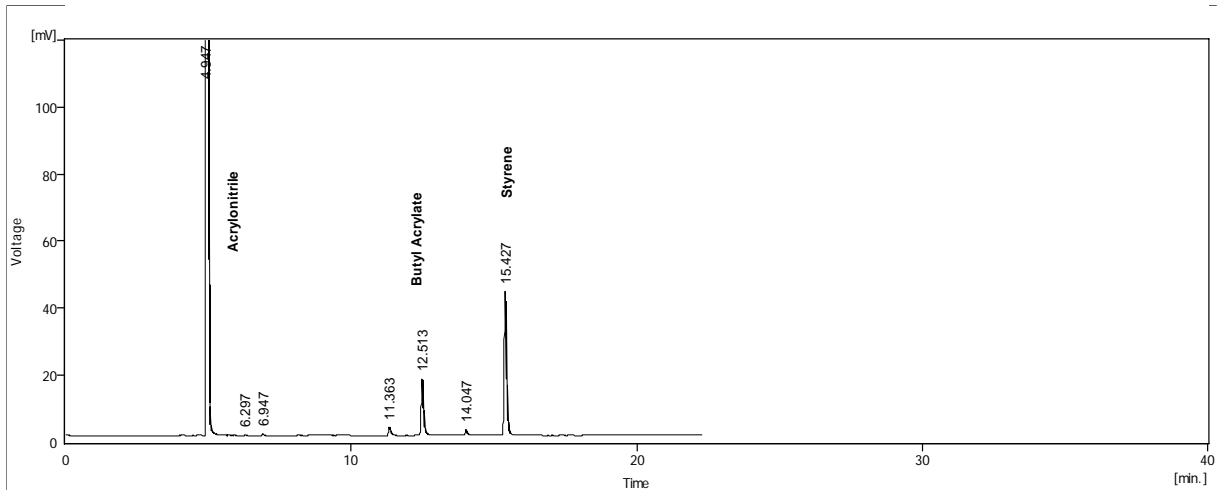
The GC-HSS method described given in the present paper can be successfully used for the determination of monomer content in acrylic polymer emulsion samples. The peaks of all the three monomers viz., Styrene, butyl acrylate and acrylonitrile from acrylic polymer emulsion samples, were clearly resolved, identified and quantified. This method can be used in the acrylic polymer manufacturing companies in their day-to-day QA /QC analytical work.

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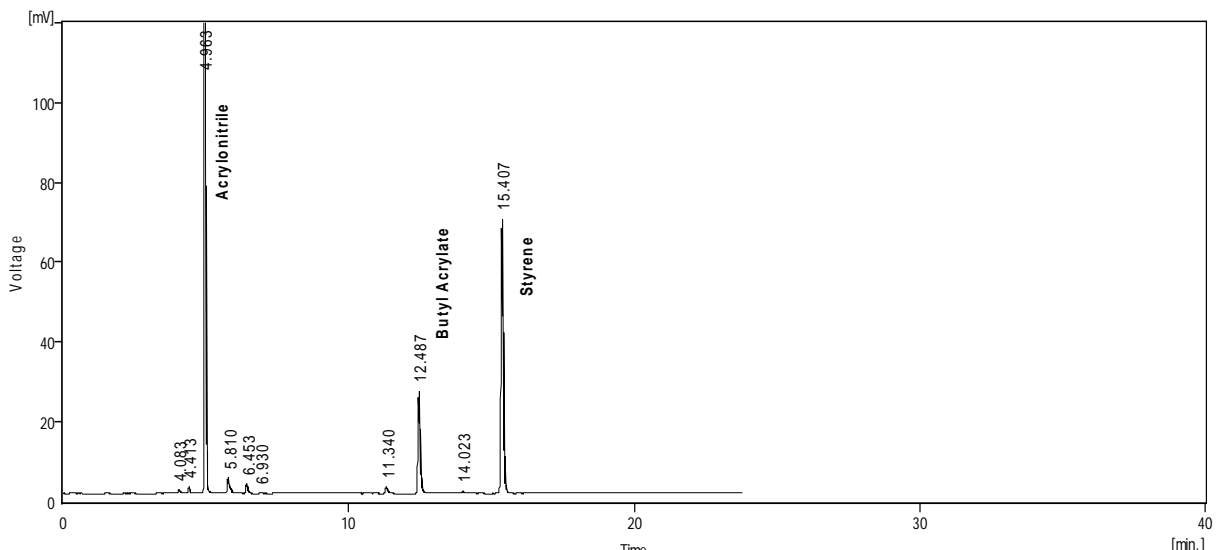
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**Figure 1: GC Chromatogram of Standard mix of Acrylonitrile Butyl acrylate and styrene**



**Figure 2: GC Chromatogram of Acrylic polymer sample No. 1**



**Table No.1: GC Analysis results indicating monomeric contents in Acrylic polymer samples**

Sr. No.	Sample Details	% of Acrylonitrile	% of Butyl acrylate	% of styrene
1.	Standard mix of Acrylonitrile, Butyl acrylate and styrene	0.5 %	0.5 %	0.5 %
2.	Acrylic polymer sample No. 1	1.7 %	0.3 %	0.16 %
3.	Acrylic polymer sample No. 2	5.87 %	0.09 %	0.11 %

#### IT-14

#### SIZE EFFECT IN SEMICONDUCTING GAS SENSORS: SOME NEW INSIGHTS

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Metal Oxide Semiconductor (MOS) gas sensors stand out as a promising class among the family of sensors, because of their simplicity and low cost. The advantages of MOS sensors are their high sensitivity to most combustible gases including saturated hydrocarbons, hydrogen, NO and CO, their fast response time and reliability, resistance to corrosive gases and the low production cost. The main lacunae of the semiconductor based thick film sensors however, lies in their high operating temperature and lack of selectivity to any particular gas. For example, though commercial SnO<sub>2</sub>-based thick film gas sensors have been available for a long time, their performance such as sensitivity, selectivity, response time and durability still needs further improvement. Hence, the development of gas sensors with optimum sensitivity and selectivity has been a major challenge in the recent years. Therefore, in order to improve the gas sensing characteristics of SnO<sub>2</sub> based materials, our recent works has mainly focussed on fabricating sensors using nanoparticles of oxides and exploit their sensitivity towards different gases. This talk would cover an overview of the processing, characterization, fabrication and properties of few selected oxides such as SnO<sub>2</sub> and CeO<sub>2</sub> and their gas sensing characteristics. Using nano particles of oxides, sensors have been fabricated for detecting butane, hydrogen and sulphur dioxide gas. The importance of using nanoparticles of oxides in developing gas sensors with high sensitivity and selectivity through selected examples will be discussed. The reduction of particle size to a dimension smaller than the thickness of the charge depletion layer has resulted in exceptionally high butane sensitivity and selectivity in SnO<sub>2</sub> based oxides. The special ability of ceria nano particles for selectively detecting SO<sub>2</sub> gas down to 5 ppm was also

observed. The *most interesting observation* from our studies is a unique combination of gas sensitivity and selectivity that has been achieved using nanoparticles without the addition of any noble metal catalysts such as Pd or Au. Thus, by controlling the particle size to the nano-regime it is possible to develop chemical sensors with high sensitivity and selectivity for a particular gas at a specific operating temperature and this is the most important observation emerged from our studies.