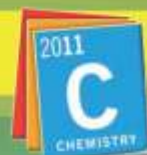
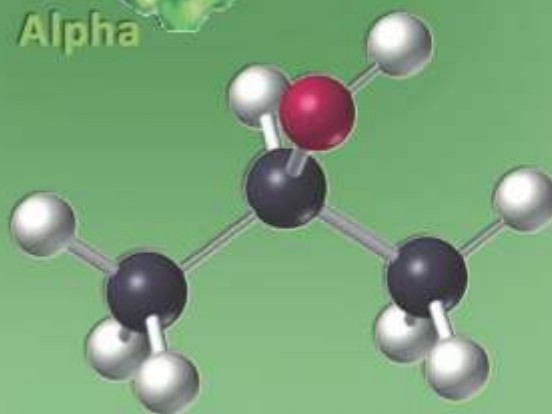
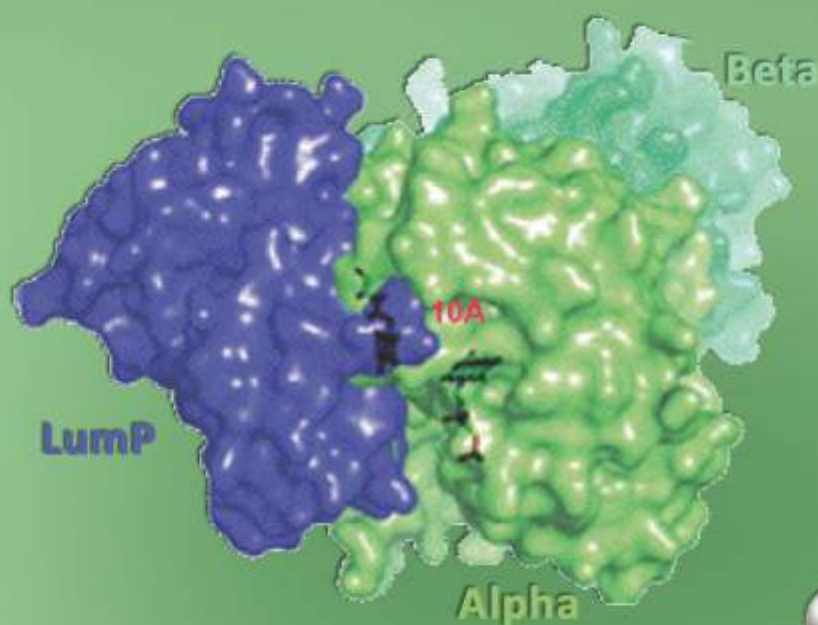


CHEMISTRY IN SRI LANKA



International Year of
CHEMISTRY
2011



Isopropyl alcohol
 $(\text{CH}_3)_2\text{CHOH}$



SEPTEMBER 2011 VOLUME 28 - NO. 3

The Tri Annual Publication of the
Institute of Chemistry Ceylon
ISSN 1012-8999

Chemistry in Sri Lanka

ISSN 1012 - 8999

The Tri-Annual Publication of the Institute of Chemistry Ceylon

Founded in 1971, Incorporated by Act of Parliament No. 15 of 1972

Successor to the Chemical Society of Ceylon, founded on 25th January 1941

Vol. 28 No. 3

September 2011

	Pages
Council 2011/2012	2
Outline of our Institute	2
Chemistry in Sri Lanka	2
Committees 2011/2012	3
Cover page	3
Guest Editorial	4
Message from the President, Institute of Chemistry Ceylon	6
Presidential Address	8
Membership News	12
Address by Chief Guest at 40 th Annual Sessions	13
Theme Seminar: Photochemistry for the wellbeing of society	
Industrial Photochemistry	15
Photochemistry and Medicine	17
Photochemistry in the atmosphere	18
Photochemical Sensors	21
40 th Annual Sessions 2011	27
Invited Articles	
Iodine in the marine environment and its chemistry in the troposphere	29
Nuclear Magnetic Resonance spectroscopy and Parahydrogen	32
Molecular Materials: Processable Forms of Polycyclic Aromatic Hydrocarbons (PAHs)	35
International Conference on Chemical Sciences	40
Call for Abstracts and Extended Abstracts	41
Report of the 40 th Annual Sessions & 70 th Anniversary Celebrations	42
Publications of the Institute of Chemistry Ceylon	43
RSC News	44

මයාලා මදර එයා හිලර -

"Role of Chemistry Research in National Development"

Adamantane House, 341/22, Kotte Road, Welikada, Rajagiriya

Office ☎ : 2861231, 2861653, 4015230

☎ : 2861231, 2861653

E mail : ichemc@slt.net.lk

web page : www.ichemc.edu.lk

Outline of our Institute

The Institute of Chemistry Ceylon is a professional body and a learned society founded in 1971 and incorporated by act of Parliament No. 15 of 1972. It is the successor to the Chemical Society of Ceylon which was founded in 1941. Over 50 years of existence in Sri Lanka makes it the oldest scientific body in the country.

The Institute has been established for the general advancement of the science and practice of Chemistry and for the enhancement of the status of the profession of Chemistry in Sri Lanka. The Institute represents all branches of the profession and its membership is accepted by the government of Sri Lanka (by establishment circular 234 of 9-3-77) for purposes of recruitment and promotion of chemists.

Corporate Membership

Full membership is referred to as corporate membership and consists of two grades: **Fellow (F.I.Chem.C.)** and **Member (M.I.Chem.C.)**

Application for non-corporate membership is entertained for four grades: **Associate (former Graduate) (A.I.Chem.C.)**, **Licentiate (L.I.Chem.C.)**, **Technician (Tech.I.Chem.C.)** and **Affiliate Member**.

Revision of Membership Regulation

All Special Degree Chemists can now apply directly to obtain **Associate (Graduate) Membership**. Three year B. Sc. Graduates (with an acceptable standard of Chemistry) can

- (i) directly become **Licentiate**
- (ii) obtain corporate membership in a lesser number of years.

Tech.I.Chem.C.

Those who have passed the DLTC examination or LTCC examination or have obtained equivalent qualification and are engaged in the practice of Chemistry (or chemical sciences) acceptable to the Council are entitled to the designation **Tech.I.Chem.C.**

Members/Fellows are entitled to the designation of **Chartered Chemist (C.Chem.)** on establishment of a high level of competence and professionalism in the practice of chemistry and showing their commitment to maintain their expertise.

All corporate members (Members / Fellows) are entitled to vote and become Council/ Committee members whether Chartered Chemists or not.

Membership Applications

Any application for admission to the appropriate class of membership or for transfer should be made on the prescribed form available from the Institute Office.

Current Subscription Rates

Fees should be paid on 1st of July every year and will be in respect of the year commencing from 1st July to 30th June

Fellow	Rs. 1200
Member	Rs. 1200
Associate	Rs. 900
Licentiate	Rs. 750
Technician	Rs. 500
Affiliate	Rs. 500
Membership for Life	Rs. 10000

Entrance Fee

All the grades	Rs. 500
Processing Fees*	Rs. 200
Processing Fee for Chartered Chemist designation	Rs. 1000
Institutional Members	Rs. 2500

*per application for admission/transfer to any grade

Headquarters Building

Adamantane House

341/22, Kotte Road, Welikada, Rajagiriya

Telephone/Fax : 2861653, 2861231

Telephone: 4615230

e-mail : ichemc@sltnet.lk

web : www.ichemc.edu.lk www.ichemc.com

Council 2011/2012

President	: Prof. S Sotheeswaran
President Elect	: Prof. S Mohandas
Vice President	: Prof. H D Gunawardhana
Immediate Past President	: Prof. M D P De Costa
Hony. Joint Secretaries	: Ms. M N K de Z Goonatilleke Dr. A A P Keerthi
Hony. Treasurer	: Mr. N M S Hettigedara
Hony. Asst. Treasurer	: Dr. (Ms) L S R Arambewela
Hony. Editor	: Prof. (Ms) Sujatha Hewage
Hony. Asst. Editor	: Dr. (Ms) Chatu Sirimanne
Secretary for International Relations	: Prof. (Ms) Siromi Samarasinghe
Chairman/Academic Board	: Prof. J N O Fernando
Hony. Secretary for Educational Affairs	: Ms. P M Jayasinha
Chairman, Admission & Ethical Practices Committee	: Mr. E G Somapala
Secretary, A & EP Committee	: Mrs Sakunthala Tennakoon
Chairman, Board of Trustees	: Prof. H D Gunawardhana

Elected Members

Prof. Sudantha Liyanage	Dr (Ms) V M Thadhani
Dr (Ms) Nandanie Ediriweera	Dr (Ms) H M K K Pathirana
Prof (Ms) Ramanie Wijesekera	Mrs D Seneviratne
Mr K R Dayananda	Dr A L Jayawardena
Dr Sisira Welliwegamage	Ms Nalini de Silva

Editorial and Publicity Committee

Prof. (Mrs) S Hewage (Editor)
Dr. (Ms) C Sirimanne (Asst. Editor)
Prof. (Mrs) Priyani Paranagama
Prof (Ms) Ramanie Wijesekera
Prof S P Deraniyagala
Prof (Ms) J Liyanage

CHEMISTRY IN SRI LANKA

Chemistry in Sri Lanka is a tri-annual publication of the Institute of Chemistry Ceylon and is published in January, May and September of each year. It is circulated among the members of the Institute of Chemistry and students of the Graduateship/DLTC course and libraries. The publication has a wide circulation and more than 1500 copies are published. Award winning lectures, abstracts of communications to be presented at the annual sessions, review papers, activities of the institute, membership news are some of the items included in the magazine.

The editor invites from the membership the following items for publication in the next issue of the Chemistry in Sri Lanka which is due to be released in January 2012.

- Personal news of the members
- Brief articles of topical interests
- Forthcoming conferences, seminars and workshops
- Latest text books and monographs of interest to chemists

All publications will be subjected to approval of the 'Editorial and Publicity Committee' and the Council of the Institute of Chemistry Ceylon.

Further, prospective career opportunities for chemists, could be advertised in Chemistry in Sri Lanka at a nominal payment. The editor welcomes from the members suggestions for improvement of the publication.

Committees 2011/2012

House, Finance and Membership committee

Prof. S Sotheeswaran (Chairman)
 Prof. J N O Fernando
 Prof. H D Gunawardhana
 Prof. M D P de Costa
 Prof. (Mrs.) S Hewage
 Mr. K R Dayananda
 Mr. N M S Hettigedara
 Dr. (Mrs) L S R Arambewela
 Mrs. M N K de S Goonetilleke
 Mr. M R M Haniffa
 Dr. A A P Keerthi
 Mr. N I N S Nadarasa
 Mr. J M Ranasinghe Banda
 Ms. Midha Masood
 Ms. Anoma Wijesuriya (convenor)

A and EP committee

Mr. E G Somapala (Chairman)
 Mrs. Sakunthala Tennakoon (Secretary)
 Prof. J N O Fernando
 Prof. H D Gunawardhana
 Prof. S Sotheeswaran
 Prof. (Mrs) Siromi Samarasinghe
 Prof. (Mrs) S Hewage
 Prof. M D P De Costa
 Dr. (Mrs) Nandani Ediriweera

Training Seminars/Workshop committee

Dr. (Mrs) L S R Arambewela (Chairman)
 Dr. (Ms) V Thadani
 Ms. Nalini de Silva
 Ms. Deepika Seneviratne
 Dr. A A P Keerthi

Board of Trustees

Prof. H D Gunawardhana (Chairman)
 Prof. M D P de Costa
 Prof. J N O Fernando
 Mr. N I N S Nadarasa
 Mr. E G Somapala
 Prof. (Mrs.) S Hewage
 Dr. (Mrs) L S R Arambewela

Library Committee

Mrs Dilmani Waranasuriya (Chairman)
 Ms P M Jayasinha (Secretary) :
 Prof J N O Fernando
 Prof S Sotheeswaran
 Dr (Ms) Vinitha Thadani
 Dr S Welwegamage
 Dr R Parthipan
 Ms Nalini De Silva
 Mr N I N S Nadarasa

DLTC Committee

Mr E G Somapala (Chairman)
 Mr R M Ranasinghe Banda
 Mr P R K Fernando
 Mr R Vidanagamage
 Mr K R Dayananda

Academic Board

Dr. J N Oleap Fernando (Chairman)
 Ms. P M Jayasinha (Secretary)
 Ms. M N K de Z Goonatilleke (Asst. Secretary)

Ex- Officio

Prof. S Sotheeswaran (President)
 Dr. A A P Keerthi (Hony Jt. Secretary)
 Mr. N M S Hettigedara (Treasurer)
 Mr. E G Somapala (Chairman, A & EP)

Members

Prof. M D P de Costa
 Prof. H D Gunawardhana
 Prof. (Ms) S Samarasinghe
 Dr. (Mrs) L S R Arambewela
 Mr. K R Dayananda
 Prof. W S Fernando
 Prof. (Ms) S Wimalasena
 Dr. (Mrs) S Iqbal
 Mr. H S M Pieris
 Prof. (Ms) Ramanee Wijesekera
 Prof. (Ms) S A Deraniyagala

Co-opted

Ms Dilmani Warnasuriya
 Mr D B N Perera
 Mr P R K Fernando
 Prof. (Ms) J Liyanage
 Dr Rohan Perera
 Prof S Liyanage
 Dr S Welwegamage
 Dr (Ms) V Thadani
 Dr R Parthipan
 Dr (Ms) R Kandiah
 Mr N I N S Nadarasa
 Mr J M Ranasinghe Banda
 Mr Y M N D Y Bandara
 Mr R Loorthurajah
 Ms S Princy

Sponsorship committee

Prof. S P Deraniyagala (Chairman)
 Prof. M D P De Costa
 Prof. (Mrs) S Hewage
 Mr. M R M Haniffa
 Mr. N M S Hettigedara
 Dr. (Mrs) L S R Arambewela
 Dr. K D P Hemalal
 Prof. (Ms) R Wijesekera
 Prof. S Liyanage
 Dr. Rohan Perera
 Dr. (Ms) C Sirimanne
 Dr. AAP Keerthi
 Mr. Arulanandasivam

Building Project Committee

Prof. H D Gunawardhana (Chairman)
 Prof. S Sotheeswaran
 Prof. M D P de Costa Prof. J N O Fernando
 Mr. H S M Pieris Prof. S Mohandas
 Dr. (Mrs) L S R Arambewela
 Prof. Sudantha Liyanage
 Mr. J M Ranasinghe Banda

Social Affairs committee

Prof. Sudantha Liyanage (Chairman)
 Mr. K R Dayananda
 Ms. P M Jayasinha
 Dr. A A P Keerthi
 Ms. D Seneviratne
 Dr. S Welwegamage
 Dr. (Ms) V Thadani

Awards committee

Prof. M D P de Costa (Chairman)
 Prof. H D Gunawardhana
 Prof. J N O Fernando
 Prof. (Mrs) S Hewage
 Prof. (Ms) Ramanee Wijesekera

Australian National Chemistry Quiz committee

Mr. N I N S Nadarasa (Chairman)
 Prof. J N O Fernando
 Prof. M D P de Costa
 Mr. E G Somapala
 Dr. R Parthipan
 Dr. R Senthilnithy

Interschool Chemistry quiz committee

Dr. A A P Keerthi (Chairman)
 Dr. R Parthipan
 Prof. (Ms) Hema Pathirana
 Dr. (Ms) R Kandiah
 Dr. A L Jayawardena
 Dr. S Welwegamage

IYC committee

Mr. N M S Hettigedara (Chairman)
 Prof. J N O Fernando
 Prof. M D P De Costa
 Prof. (Mrs) S Hewage
 Prof. S P Deraniyagala
 Prof. S Sotheeswaran
 Prof. (Mrs) S Samarasinghe
 Dr. (Mrs) N Ediriweera
 Dr. (Mrs) Arambawela
 Dr. A A P Keerthi
 Prof. (Mrs) J Liyanage
 Prof. K R Mahanama
 Mr. K R Dayananda
 Mrs. M N K De S Goonethilake
 Ms. D Attanayake
 Mr. N I N S Nadarasa
 Mr. J M Ranasinghe Banda
 Mr. A M Jayasekara

Monograph Committee

Prof. M D P de Costa (Chairman)
 Prof. S P Deraniyagala
 Prof. Ramanee Wijesekera
 Prof. P Paranagama
 Prof. (Mrs) J Liyanage

Cover Page

Lumazine protein (LumP, blue) associated to the alpha subunit (green) of bacterial luciferase) revealing a 10 Å^o separation between the lumazine binding site on LumP and the flavin-active site of luciferase.

See pages 21 - 26.

Chemistry Education in Sri Lanka: Are we on the right track?

Professor H D Gunawardhana

Part time Senior Professor, College of Chemical Sciences, Institute of Chemistry Ceylon



In the older concept, a chemistry teacher is a person who transfers the knowledge (skill) to the student. In the modern concept, this is inadequate unless the transfer of knowledge assists the student to develop the competency in the subject matter taught. It is the duty of

the student to develop the competency to use the knowledge when requires. The teacher will facilitate the students to develop their skills which involve the ability to apply the knowledge when the need arises to real systems rather than the traditional imaginary examples. The evaluation process should be based on the award of credits to those students who develop the capability to apply scientific principles to the industry.

In the traditional method, scientific principles are taught by applying mainly to imaginary examples. The skill is developed by carrying out the laboratory work. It is essential that a student will develop the ability to apply chemical principles to technologies in Sri Lanka. There is a dearth of personnel who possess this ability (less than 10 % - "scientific literacy"). In the modern concept, a teacher is a facilitator who will guide the student to develop the so called "scientific literacy". Following question was given to forty graduates from Sri Lankan Universities and tertiary educational Institutions who offered chemistry as a subject: Give the reason why copper(I) with----- $3d^{10}$ electronic configuration is unstable and easily oxidized to more stable copper(II) ----- $3d^9$ whereas silver(I)----- $4d^{10}$ is stable and silver(II)----- $4d^9$ is not common. A clue was given that copper(I) sulphate (white crystals) turns blue in Sri Lanka having over 90% humidity but in countries where the humidity is low white copper(I) sulphate can be kept for a longer period. The theory required to give a satisfactory explanation has been done in the inorganic chemistry area. It was unfortunate that not a single graduate was able to produce the correct answer which involves correlation of the theory with the laboratory observations. This is also true for the applications of chemical principles to technologies. It is not possible to deny the statement by industrialist that "graduates are useless, they cannot think".

Over 90% of Sri Lankans possess the ability to use the language of words. Similarly, over 90% of students who learn chemistry as a subject possess the ability to reproduce the subject matter as it is. Should

we claim that the 'literacy' of chemical education is over 90%? The chemical education is the transfer of knowledge / skill in chemistry from the teacher to the student. The transfer is inadequate if the student does not possess the ability to use the knowledge/skill when requires. The ability to use the knowledge/skill in chemistry when the need arises is considered as the 'literacy' in chemical education. An average student will not automatically develop the ability to use the knowledge/skill when the need arises unless he practices. It is like any other activity in life e.g. driving a car a student has to practice to develop this ability. The most important way that an average student will develop this ability is by 'self learning' after the knowledge is transferred from the teacher. The best self learning is the reading of text-books. An average student may require to read the text-books several times to achieve proper understanding of the principles he learnt. Even though the time required for such a process varies from student to student it will not only be helpful for student to gain a better knowledge in chemistry but also be useful to acquire the ability to use the knowledge in chemistry when the need arises. Since it is a very slow process it has to be initiated at least at the secondary level of education. A student who has undergone the training of this self-learning practice, after the completion of his learning of chemistry will be a citizen who possesses a great potential to contribute towards economic development of the country.

Is the 'literacy' in chemical education achieved today? Today the self-learning aspect of chemistry is not popular among the students who read chemistry as a subject due to,

- (i) the inadequacy of reading materials in chemistry written in the language of instruction, and
- (ii) the popular examination oriented study prevailing among students who only study the answers to a particular set of questions.

In order to achieve the National Goals the curriculum at G.C.E.(A/L) should cater for 95% of the students who do not gain admission to Universities in Sri Lanka. At present, the course content in chemistry is geared for the minority (5%) who pursue higher education. In many developed countries, the authors who have published books for the Secondary level are not allowed to participate in the designing or the revision of the course content. This is because the vested interest inadvertently predominates over the National interest. Since there

is no such rule in Sri Lanka the students who offer chemistry at G.C.E. (A/L) do not find any usefulness of the subject if they fail to gain admission to the Universities. Sri Lanka suffers because the vested interest predominates over the national interest. A frequent revision of the curricula is essential to suit rapid changes in some aspects of chemistry. It is suggested that a permanent body should undertake revision of the curriculum of chemistry at G.C.E. (A/L) after conducting research on the aspects of catering for 95% of the students. This is cost effective since it helps in the development of the economy of the country. Even though there are about 35,000 irrigation tanks (WEWA or VARI) the irrigation water quality is not in the curriculum. Since there are no irrigation tanks in UK and USA their curricula do not have irrigation water quality. Whenever an attempt to incorporate irrigation water quality to curricula it became futile due to the fact that it does not fall with the curriculum of UK.

It is true that ancient Sri Lankans did not have the so-called modern science which is not more than 500 years old. The ancient technology was based on unwritten science (traditional wisdom), and is not the

modern science. The survival of the ancient technology was possible for several years due to its association with this unwritten form of science which would have been in some cases a kind of family secrets. The survival of technology is dependent on science. The economic development through agriculture in ancient Sri Lanka was due to the application of 'Sciences' (traditional wisdom) to the technological needs during that period. The sustainable development achieved during the ancient time was completely ignored or disregarded. Often, the concept of sustainable development is taken as a modern invention. In fact, it is a concept regarded as a part of our ancient culture. It would be fruitful for us to have some understanding on the application of unwritten science to ancient technology in order to achieve economic development by the application of modern science which is familiar to us now due to existing technology. Since "Education determines the economy of a Country" there is a need to educate our children or even all stake holders including teachers on the importance of Science for sustainable development.

Benevolent Fund Benefits for Members

- **Long life** Benefits: Rs. 10,000 (over 70)/Rs. 15,000 (over 75)/Rs. 20,000 (over 80)
- **Critical illness** benefits (upto Rs. 50,000)
- **International travel** for conferences (upto Rs. 50,000)
- **Balance 50% of Tuition fees** of any member's child following the Graduateship Programme (Since 50% concession is already by CCS, this will amount to a 100% waiver)

Any member who has paid membership fees for life (after 3 years of such payment) is entitled for these benefits. All members are advised to pay the membership fee for life and become beneficiaries.

Eighth CCS Convocation

The Eighth Convocation will be held on 16th February 2012 (Thursday) at **Waters Edge**. **Mr. Susantha Ratnayake**, Chairman/CEO of John Keells Holdings PLC will be the Chief Guest. He is also the Chairman of many listed and un-listed companies. He is a Council member of the Employers' Federation of Ceylon, Chairman of the Ceylon Chamber of Commerce as well as the Chairman of the Sri Lanka Tea Board.

IYC Open days & Exhibition



To further commemorate the IYC, an Open Day & Exhibition will be held on **November 24, 25 & 26** at Adamantane House. College students will conduct various activities such as A/L Chemistry practical presentations and exhibit pharmaceutical chemistry, environmental chemistry & food chemistry stalls. There will also be training seminars, titration competitions, chemistry magic show etc. The main objective of the open days is to popularize chemistry particularly amongst school children. The **Inter Level Debating Competition** will also be held. More events are being planned

Message from the President, Institute of Chemistry Ceylon

The year 2011 is special for chemists because it has been declared the International Year of Chemistry (IYC)—2011 by the United Nations Organization. The attention grabbing slogan “Chemistry—Our life, Our Future” pithily expresses the importance of chemistry in our life and the crucial role it has to play in the future. If Chemistry is central to our life, it goes without saying that chemists and the educational institutions and curricula that produce chemists are important.

For some years now in Sri Lanka, those involved in the field of education have been wringing their hands and helplessly repeating that there are employers looking out for workers and that there are unemployed people looking for jobs but never the twain meet with mutual benefit and satisfaction. Are our educational institutions producing unemployable products?

Today there is a great mobility of workers globally. It is common knowledge that some job vacancies in Sri Lanka are being filled by foreign workers. It is also true that today there are all kinds of unusual and new jobs in Sri Lanka that were unheard of say 50 or even 25 years ago. The great need is to devise and popularize courses and programmes of study that will produce employable workers.

Ambition is a good thing, but what do we do with the thousands of A/Level students who yearn to become doctors or engineers and are frustrated when they do not gain entry to the faculties of their choice in state universities even after doing the A/Levels three times? Some of them spend enormous sums of money overseas, and return home having trained as doctors in Czechoslovakia, Bangladesh, Nepal and so on only to find that they cannot find employment here because the job vacancies are limited. I understand that there are many unemployed doctors, who received their medical training in foreign lands. These are hardworking and highly motivated students. It is a pity they did not divert their talents to other fields.

Chemistry is not only a central science (necessary for medicine, dentistry, veterinary science, chemical engineering, agronomy, pharmacy, nutrition and so on) it is also a versatile science. A chemist can fit into a wide variety of jobs. We at the Institute of Chemistry have done our part to popularize chemistry. Mention must be made of the extra effort made by many to seize the opportunities offered by IYC—2011 to raise awareness among the public and secondary school students of the opportunities offered to chemists to better their own prospects and to serve society and our country. Special mention must be made of CHEMEX—2011, an exhibition held this year from January 27-29 at the BMICH, Colombo. The exhibits and activities provided were wide and varied, and the response from the public and students was overwhelming.

The Institute of Chemistry is justifiably proud that its educational arm, the College of Chemical Sciences, has produced professional chemistry technicians and graduates for about 40 years. Students who have gone through the College of Chemical Sciences are our best ambassadors. Many of them have done us proud locally and internationally. The industry and enthusiasm of our students keeps the staff on its toes. Courses are revised and new courses are added to keep abreast of developments in Chemical Education and the demands of the job market. As the honorary Rector keeps pointing out, the significant and praiseworthy contribution that the College makes in educating chemists is no financial burden to the national exchequer.

We have no intention of resting on our laurels. The College has grown beyond anyone's expectations from small beginnings. It will continue to provide quality education in the field of Chemistry.

Research is a part of the training provided at the College of Chemical Education as it is in the universities.

Research that is relevant to and appropriate for Sri Lanka will surely find applications that will benefit society and our country. We hope to foster this.

I appeal to members of the Institute of Chemistry to recruit new members, especially young technicians and graduates. We need young and energetic members to carry on the good work of the Institute.

Prof. S Sotheeswaran
President, Institute of Chemistry Ceylon



Prof S Sotheeswaran was ceremonially inducted by the President, Prof M D P De Costa, as the new President for 2011/2012 by awarding him with the President's medal.

With Best Compliments From

Techno Instruments (Pvt) Ltd

**THE BEST OF THE BEST IN
TEST & MEASUREMENT AND LIFE SCIENCE &
CHEMICAL ANALYSIS PRODUCTS**



Agilent Technologies

Authorized Distributor



TECHNO INSTRUMENTS
(Pvt) Limited

No.25, Rajawatte Terrace, Siebel Avenue, Colombo 05, Sri Lanka

Tele: +94 11 2820192, +94 11 2820194

Fax: +94 11 2823653

Email: techins_1@sltnet.lk / technis_2@sltnet.lk

Chemistry and Society

Professor M D P De Costa

Department of Chemistry, University of Colombo

Introduction Chemistry

Chemistry is a broad science. It deals with the concepts of creation of molecules and the manipulation of atoms at both microscopic and macroscopic scales. The 20th century has seen the birth of three Ages, each with profound social implications. These have been called the Nuclear Age, the Electronic Age and the Chemical Age. The latter is the oldest (beginning around 1930), and although its impact has been less dramatic than the other two, its consequences have more thoroughly and deeply affected our day-to-day lives. Our local grocery, hardware and drug stores carry an impressive array of commonly used chemicals, such as detergents, adhesives, lubricants, fabrics, pesticides, fertilizers, pharmaceutical drugs, vitamins and a multitude of fabricated plastic items. **Chemistry affects the people of our planet, protecting and preserving our health, ecology, culture and heritage.**

While chemistry is a science in its own right, it also supports and interacts with other scientific disciplines. Chemistry along with biology, physics, medicine, materials science and other core disciplines, makes effective contributions to the solutions of problems facing the world today and to the improvement of the condition of mankind tomorrow. In leading technology towards the future, it should be remembered that chemistry is not a new science, but a steadily evolving discipline like physics and biology, interdependent on discoveries in other areas. It is a discipline that has long and deep traditions in the world. **Chemistry is responsive to the challenges of the world economy, environment and culture and to the influences of scientific discovery.**

Society

Society consists of groups of people in various living conditions and different age levels. All of them need proper education, good health, medicine when they are sick, entertainment, food to eat, water and other beverages to drink. Society as a whole was undergone tremendous hardships to achieve some of the basic needs in life. Life expectancy and the comfort factor were very poor. Chemists have developed many things for the betterment of life. Development of new

materials and medicine and improvement of food quality, development of new methods for harvesting and storage are a few examples. **For continuous development we have to take steps to educate the society and specially our young people in Chemistry.**

Chemistry & Education

Schools provide for teaching young children the basics of chemical sciences starting from the O/L through to the A/L. Universities including College of Chemical Sciences (CCS) provide teaching and training for bright young people in the basic and advanced chemical sciences. Universities and CCS have a vital role in the training of people and as partners with industry in collaborative research and development. Universities and CCS send their students to undergo training in Industry. The trained chemists needed for Industry and Research Institutions in Sri Lanka depend only on Universities and CCS.

Of course, provision of an educational training in chemistry does not begin at university. It starts at primary school with an introduction to observation and interpretation of phenomena, and continues through early, middle and later schooling. There are deep worries within the chemistry community in Sri Lanka that the educational provision in science is lacking in appropriate resourcing and basic training and particularly in mathematical and soft skills.

Schools and universities have a major contribution to make in improving society's knowledge of chemistry and chemical technology. Chemistry teaching must be better funded and empowered through better training to deliver higher standards in chemistry education. Education must continue for our workforce throughout the working life. Chemistry education must be seen as a fundamental basis for a modern society. Better teaching in Chemistry is always dependent on the practical experience in fundamentals and principles in Chemistry. This is lacking in the Sri Lankan education system. Unfortunately the student's knowledge in Advanced level chemistry is coupled with university entrance. Therefore, students strive hard to learn the chemistry required answering questions rather than to applying the concepts learned. This leads to a situation where the learning of Chemistry is limited to good grades at examinations. The benefit the country could

get from chemistry educated children will be suppressed to a great extent due to this unfortunate situation.

It is very important to develop methods and chemicals to uplift the living standard of society. Therefore it is necessary to develop industrial research to a higher level. Those who learn chemistry should be able to participate actively in such research and apply their skills to uplift the quality of industrial products and develop new materials.

Chemistry & Industrial Research

Industrial research is the key to developing the economy of a country. Therefore the new products which give solutions to problems in existing product are found, leading to a more comfortable life. In most countries, universities have collaborative research with industry. But this collaboration is lacking in Sri Lanka. The chemical industry of the world has grown to its present importance through a steady stream of innovation in products and processes. Many new ideas, concepts and techniques come from continual contact with fundamental and applied research in chemistry and chemical engineering. These provide the intellectual driving force of innovation. Without research in chemistry and chemical engineering there would be markedly fewer improvements in the quality of life. Unfortunately this is very much lacking in Sri Lanka. Many of our university academics have tried their best to interact with industry to develop such collaborative research. Due to the rules and regulations of public universities and private sector industries such collaborations have become weak and the interest of both parties has declined. Government dependent research institutions play a bigger role in Industrial research. However, collaboration and support from the universities are lacking due to various reasons. At present only university students carry out their industrial training at such research institutions and private sector industries. This has also been affected a great deal due to various reasons. Most of the Research and development in our industries is carried out on a small scale may be due to the small market we have in Sri Lanka. But our industries must target the world market and only quality products can reach that level. Therefore continuous research and development must be carried out by Industries in Sri Lanka to achieve such high standard. Chemistry laboratories in universities and research institutes need adequate provision of

instruments through local and national facilities. They also need modern laboratories, equipped to modern safety standards, to conform to good practice in the training of researchers. Recently the University of Colombo established a Research and Development laboratory for the pharmaceutical sector with the help of a government grant. This will help to upgrade the quality of drugs produced by Sri Lankan pharmaceutical companies. Such laboratories are essential and continuous government and private support is necessary to establish them. Universities can provide knowledgeable human resources. **This will definitely enhance the effective use of higher education in Chemistry among the university students.**

Chemistry and Higher Education

The facilities available in Sri Lanka for higher studies are very limited. This results in most of our outstanding students who learn their chemistry through universities and CCS, going abroad for their higher studies. Unfortunately majority of these people do not come back and there is big vacuum for skilled personnel in Sri Lanka. This is mostly due to the better opportunities they have in other countries and the poor treatment they get in Sri Lanka. The development of industrial research and attracting graduates to industry by offering them an opportunity to obtain a higher degree in collaboration with universities may help retain some of our students in the country. Industries and Universities have a big role to play in this regard. Better laboratories at Industrial and National levels must be developed. The government and private sector have an important role in funding these activities.

Impact of Chemistry Education in Industry

Chemists and chemistry students are trained to design, optimize, and evaluate chemical synthetic pathways based on the selectivity and/or yield of a reaction step. Yield is the percentage of actual products obtained versus the theoretical amount which could be obtained from a given amount of reactants at specified conditions. It is an important indicator of how efficiently chemical feedstocks and other reaction inputs can be utilized in a reaction step. Efficient use of chemical feedstocks inevitably increases the cost effectiveness of a reaction or synthetic pathway. Coupled with the cost of feedstock

materials and energy consumption, reaction yield is one of the fundamental performance criteria for chemists to evaluate the industrial-scale feasibility of chemical reaction pathways.

Until recently chemists focused very little on the toxicity of feedstocks or the by-products of commercial syntheses. In addition, chemists' concerns about reaction media and reaction pathways were narrowly focused on use of traditional organic solvents and reducing the number of steps in a particular pathway. Similarly, when chemistry students are taught to synthesize and/or isolate chemical substances, their thought process is not structured towards consideration of health and environmental consequences of reaction pathways. Therefore students need to be aware that decisions to utilize, generate, and dispose of hazardous substances are made intrinsically through selection of specific reaction inputs. In addition, they must learn to evaluate the upstream and downstream impacts of design decisions related to chemical synthetic pathways.

Chemistry and the Environment

In the past scientists concerned themselves with solving visible problems in society, such as easing poverty and disease, traveling faster, making our lives more convenient. The environment was considered a source of natural resources which should be exploited to fuel societal development. Chemistry was viewed as a scientific tool which could harness natural resources to enhance our lives in these ways. This attitude was reflected by the following marketing slogan used by DuPont Chemical Company prior to 1970: "Better things for better living . . . through chemistry". Unfortunately, in providing solutions to our immediate needs in society, scientists sometimes created more complex problems with large scale impacts. The production, processing, and use of chemicals in modern society have been accompanied by global-scale environmental pollution, natural resource depletion, and health impacts. In some cases the implications of such impacts were masked due to a superficial scientific understanding of an inability to measure the fate, transport, and toxicity of chemicals in the environment. Concerns regarding the safety of a chemical product were potentially addressed in terms of immediate and/or microscale impacts. However, long-term and/or global impacts of chemical use on environment and health were not necessarily of

significant concern to scientists, regulators, and the public. The depletion of the stratospheric ozone layer by chlorofluorocarbon chemicals (CFCs) and the bioaccumulation of chlorinated organic pesticides in the food chain demonstrate the need for a more comprehensive consideration of the potential impacts of chemical use in society.

For almost 50 years CFCs were considered the best chemical due to their low acute toxicity and non-reactive nature. Their competitive production cost made them an ideal candidate for numerous industrial and consumer applications. This includes their use as refrigerants, propellants in aerosol cans, in hospital sterility, as industrial solvents, and foam blowing agents. Worldwide use of CFCs increased from 400 million pounds in 1960 to 2.5 billion pounds in 1988. In 1974 atmospheric chemists Mario Molina and Sherwood Rowland published data which suggested that CFCs could have a significant role in the depletion of the stratospheric ozone layer. These scientists encountered considerable skepticism from fellow chemists, government regulators, and the general public. However, their theory was confirmed in 1987 when other scientists definitively linked the chlorine component of CFC molecules to the destruction of ozone molecules in the stratosphere above Antarctica. Chlorinated hydrocarbon pesticides, such as dichlorodiphenyltrichloroethane (DDT), were first introduced for use in chemical pest management in the 1940s. Their effectiveness in eradicating pests and vector-borne diseases, such as malaria, typhus, and yellow fever, made these chemicals, "wonder chemicals" for agricultural and public health programs. Applications of DDT during World War II were responsible for making this conflict the first in history in which more combatants died from direct effects of war rather than epidemic and endemic diseases. In 1962, Rachel Carson published her controversial text, "Silent Spring," which provided both scientific and subjective evidence of the negative effects of bioaccumulation of chlorinated organic chemicals in the food chain. As was the case with CFCs, scientists in government and industry initially discounted the hypothesis of Carson's book. However, many of her observations were indeed valid. It was later discovered that DDT and other chlorinated organic chemicals bioaccumulate in the fatty tissue of non-target species at the head of the ecological food chain. The development of CFCs and DDT exemplifies the beneficial and destructive impacts of chemical

production and use in society. It also demonstrates the unsafe position which all scientists hold in our society. There are many more chemicals developed by scientist that have the same beneficial and destructive effects towards society.

Chemists are expected to fulfill our demands for innovative products. However, they also face sharp criticism for a perceived disregard of the environmental and health impacts of their work. The scientists who developed CFCs and DDT probably did not have the knowledge to predict the long range adverse impacts associated with these chemicals. Their research efforts focused on the development of less toxic chemical products with specific functional properties. However, the unexpected long-term impacts of their production and use demonstrates a clear need for scientists to develop a broader set of considerations in the initial design phase of chemically based products. What could we expect from genetically modified and nano-scale materials in the future???

Role of Chemist for the Better Future of Society

How will chemists of the future balance competing concerns of environmental friendly and innovative, cost-effective product development? For chemists to accept the idea that environmental quality and economic prosperity can be intertwined, it is very important to have an understanding of the environment fate of chemicals and their processes. These must first be integrated into their underlying thought process. Chemistry students need to understand the complexities that health and environmental concerns bring to a particular chemical synthetic pathway. They must consider them no different than traditional concerns of yield, reaction selectivity, and stereo-specificity.

Such knowledge is just as critical for introductory chemistry students as it is for those enrolled in more advanced chemistry classes. In Sri Lanka less than 2% of all students who follow science in school enroll in university-level chemistry courses. However, these courses do not have a significant and lasting effect on a student's approach to an understanding of the discipline. The number of people in society who understand the use of chemicals and their impact on the environment is insignificant. Their knowledge of chemical sciences is reflected in their daily decisions as consumers in our society. A meaningful question to ask is what should chemistry educators be teaching their students to enable them to understand and form

appropriate responses to global-scale impacts of chemical production and use. Most of our universities offer Environmental Chemistry courses. The University of Colombo in particular offers a course named Impact of Chemistry on Society to undergraduates. I believe that chemistry students should have a basic understanding of the following subject areas in order to adequately address environmental and health considerations in their own field of study: biology and biochemistry, risk assessment and statistical modeling, economics and management, politics and sociology, media and communications, and ethical perspectives.

Ethical and philosophical questions are a part of the foundation of all scientific study. Chemical science principles are applied by scientists to define the physical and biological outcomes that occur as a result of chemical production and use in our society. However, chemists are not necessarily trained to weigh the "value" of a chemical to society versus its inherent impact on the biosphere. Chemistry professors, as both scientists and educators, have an obligation to impart both ethics and knowledge through their teaching. As Vellaccio states, to teach chemistry any other way is like, "teaching someone to use a gun without teaching them the responsibilities that go with that knowledge,". Traditional chemistry curricula currently fail to train students with the appropriate multi-disciplinary background and skills necessary for them to make such decisions in an unbiased and educated manner. Educational institutions must therefore make changes in the methodology in which they educate chemists.

Such enormous changes are not made by simply telling students to avoid using hazardous reagents, solvents, or reaction conditions. Analyzing the potential of a chemical reaction requires the utilization of scientific and non-scientific parameters to balance societal costs and benefits. Such analyses are complex, uncertain, and subjective. However, government regulators, employers, and the public will expect innovative chemists to incorporate these principles directly into their decision-making processes in the future. It is the responsibility of the academic establishment to provide chemistry students with an appropriate educational background, which incorporates these concepts into their training and fosters the development of multi-disciplinary, informed decision-makers.

I strongly believe that the following changes should be made in order develop our country

economically and to raise our living standards without damaging the environment.

1. To decouple the school education system and examinations from university entrance examinations.
2. To establish strong interactions between universities and industries.
3. To establish laboratory facilities, for industrial research to be carried out in collaboration with universities and obtains government funding for

such activities.

4. To establish collaborative research programs in industry that enable our young chemists to carry out their higher studies in Sri Lanka.
5. Providing better treatment for those who are remaining in the country for the development.
6. To incorporate importance of environment fate of the chemicals we use to comfort our life to the curriculum of school education.

Membership News

The following persons have been either transferred or admitted to the categories of membership and designation between May 2010 to July 2011.

Admission to Chartered Chemists

Dr. H P Gunawardena, Mr. S De Silva, Mr. W S D Jayasena

Transfer to Fellow

Ms. L D A Wickramanayake, Mr. P G Madawala, K Abeygooneratne

Admission to Fellow

Mr. D H L W Jayamanne

Transfer to Member

Mr. A A P N Perera, J I P Perera, Mr. S A S Koswatta, Ms. D U D Rajapakse, Ms. R A D R Gunawardena, Ms. S P D S Gajaweera, Ms. P G L A Samaranyake

Transfer to Associate

Dr. S H Nilar, Mr. A J S Chinthana

Transfer to Licentiate

Mr. J P R P Premalal

Admission to Member

Dr. H P Gunawardena, Ms. N Nizam, Mrs. K A D S Mallika, Mr. E A Edirisinghe, Mrs. K V Ratnapala, Mrs. E G Lokumudaliyage, Ms. A P Attanayake, E S J Rathnaweera, H N Kodikara, A D J D D Dharmadasa, M M S Bodamuna, H M A P Herath,

Admission to Affiliate

Mr. D M E L Dissanayake, Ms. F R Mansoor

Admission to Associate

Mr. A N Madusanka, Ms. H M K Hippola, Ms. G P W Silva, Mr. W M K J Weerasingha, Ms. W C I Cooray, Ms. E D C P de Alwis, Mr. W A M Harinda, Mr. R A S D Jayawardhana, Ms. N P W Rathuwadu, Mr. K H P R de Silva, Ms. L R Gurusinghe, Ms. P G D Kaushalya, Ms. F N Ashan, Ms. K T P M Ahugammana, Mr. Y M N D Y Bandara, Ms. M L C Coorey, Mr. G J V Dabera, Mr. J V A Dahanayake, Mr. W S de Silva, Mr. S C D Fernando, Mr. S D J Fernando, Ms. W B M L Fernando, Mr. S S Gajaweera, Ms. H M D T Herath, Ms. H H S Y H Hewawasam, Ms. L R S Jayasinghe, Ms. A S K Kankanamge, Ms. B I Karawadeniya, Ms. J M D K Karunaratne, Mr. S Loganathan, Mr. R Loothuraja, Ms. D S D W Madanayake, Ms. K A N K Manathunga, Ms. A S S M Endis, Ms. K M Nagawatte, Ms. C H Narangoda, Ms. N K B S S S K Narasinghe, Ms. S Nilushni, Ms. K M Rajapaksha, Mr. U P M Shavinka, Ms. P A I C Silva, Ms. S M R W S Silva, Ms. N Sivanantha, Ms. D Sriselvam, Ms. T V M Sriyanjani, Ms. C B Thanganayagam, Ms. H L T Udayakanthi, Ms. M S K Wanigasekara, Ms. W A C V Warsapperuma, Mr. K B W M R A I Wathupola, Ms. R D P M Weeraratna, Mr. W B A Wijayarathna, Ms. A U Wijesekara, Ms. G U Chandrasiri, Ms. R A D U Ranawaka, Ms. W M U D Bandaranayake, Ms. S L O Erandika, Ms. D L Basnayake, Ms. D N Dasanayake, Ms. K K D P M Dhanapali, Ms. D M T P Alwis, Ms. S A K Amarasinghe, Mr. S Senthil Maaran, Ms. H S M Fernando, Mr. W H A K A A Buddhapriya, Ms. A G M J Gunaratna, Ms. M C N Fernando, Ms. H D Hansamali, Mr. B M D Senevirathne, Ms. P A N K P Jayawardhana, Mr. H A G S Perera, Ms. N C Abeyasinghe, Ms. F Z Z Mohamad, Mr. V D Suaris, Mr. S Mithurshan, Ms. K A D M S Sarathchandra, Mr. M R R Prabhath, Mr. G W C S Perera

Admission to Licentiate

Ms. D M Abeygunawardhana, Ms. K A C M Dulshika, Ms. L C S Wanigasooriya, Ms. M K G Morawake, S Saravan, Mr. J M S L Jayasundara, Ms. I Warushawithana

Admission to Technician

Ms. D Y Y W Dasanayake, Ms. F S Mufthi, Mr. S Kirupairajh, B Selvendran, M N F Shifana

Better Living through Chemistry?

Professor James A. Pincock

Professor in Chemistry, Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada

When I received the invitation from Professor M.D.P. De Costa to be the chief guest at the 40th Annual Sessions of the Institute of Chemistry Ceylon, I was very pleased to accept for several reasons. First, I appreciated knowing that I was considered suitable to receive such an honour. Second, it was a chance to renew my friendship with him, a former student whom I supervised at Dalhousie University (Ph.D., 1990). During that time, as well as in two later visits while he was on academic leave, he made major contributions to my research program that resulted in several very significant publications. Finally, we welcomed the chance to come to Sri Lanka, a country that my wife and I have always wanted to visit. So far, we have not been disappointed by that decision.

The city of Halifax in the province of Nova Scotia, where we live, could be a sister city of Colombo – both are seaports, both are capital cities (Halifax of the province, Colombo of the country) and both a home to major universities. The obvious differences are the climate and the population; the entire population of Nova Scotia is only about one million while that of Sri Lanka is about 20 million. Both these differences were obvious as soon as we got off the plane!

By coincidence, this year is also the International Year of Chemistry (IYC), an initiative of IUPAC and UNESCO, with the unifying theme “Chemistry – our life, our future”. The four goals of this initiative are to:

1. increase public appreciation of chemistry
2. encourage interest in chemistry among young people
3. generate enthusiasm for the creative future of chemistry
4. celebrate the contributions of women to science at the 100th anniversary of the Nobel Prize to Marie Curie.

In my opinion, major progress is being made in the fourth of these goals. For instance, my graduating class in 1965 consisted of 16 males and one female; the graduating class last year at Dalhousie, my current university, consisted of 12 males and 22 females. Clearly, women will play a major role in chemistry in the future. Perhaps they will contribute to providing a more thoughtful, humane approach to chemical usage.

So – why the title of this presentation? As I remember, it occurred to me while I was considering the IYC goals. The question mark in the title is to emphasize the ambiguity about the historical role of chemistry in society. Chemists are of the opinion that huge advances for the public good have been made as a result of their contributions. The public is not so sure.

“Better Living through Chemistry” – I had always

thought that this phrase was the motto of the Dupont Chemical Company. However, that is not so. Their actual motto was originally “Better Things for Better Living – Through Chemistry”, conceived in 1935. In 1982, this was shortened to “Better Things for Better Living” and in 1999 was changed completely to “The Miracles of Science”. Notice, that the word “chemistry” was dropped, possibly for public relation reasons. Perhaps not all of the miracles proved to lead to better living. In fact, the title for this presentation first appeared in popular culture as a song title referring to the use of recreational drugs (Fat Boy Slim) and in the movies (Batman).

Actually, the history of the Dupont chemical company clearly indicates the dichotomy that I am attempting to illustrate. Many of their products have had positive effects on society (new materials such as the polymers, nylon, neoprene, Teflon, freons, Tyvec, Kevlar, etc.). Some, such as chlorinated fluorocarbons (CFCs), however useful, were shown to have detrimental effects on the environment. In fact, in 2007, Dupont was ranked as the largest producer of air pollution in the United States by the Political Economy Research Institute of the University of Massachusetts.

To exemplify the ambiguity in “Better Living through Chemistry”, I have chosen malaria, a disease well known in Sri Lanka. In 1946, 2.8 million cases were reported in this country; in 1963, only 17 cases were reported! The difference – the extensive use of DDT. DDT was first synthesized in 1874 and, considerably later, was found to be a potent contact insecticide for mosquitoes and other insect pests by Professor Paul Muller (Nobel Prize in Physiology or Medicine, 1948). It proved so useful in this regard that between 1950 and 1980, 40 million kilograms per year were being manufactured for agricultural use, mainly in the United States. But the accumulation in the environment had a significant negative impact on other species, particularly birds, including America's national symbol, the bald eagle. In 1962, Rachel Carson's book “Silent Spring” brought public awareness to the potential fallout and was one of the factors in the emergence of the environmental movement. In 1972, the production and use in the US was banned. By then, however, as a result of its use, malaria in the US had been totally eradicated – not so in many other tropical zones, particularly sub-Saharan Africa and including Sri Lanka. This dichotomy in the use of DDT prompted R. Gwadz of the US National Institute of Health to state in 2007 that “the ban on DDT may have killed 20 million children”. In fact, a high risk of malaria now exists only in tropical

countries with lower standards of living – “balancing risks on the backs of the poor” (Nature Medicine, **6**, 729, 2000). Fortunately, current clinical trials indicate that a non-chemical solution may be imminent with the development of an antimalarial vaccine.

The negative aspects of chemistry are fodder for often sensationalized reports by the media. As a result, the public now tends to equate “chemicals” with often unnecessary and sometimes harmful additives. In the current popular view, anything “chemical” is unnatural, and anything natural has no chemicals. Few seem to realize that everything in the world, good or bad, is composed of chemicals. Thus the comments by Nicole Moreau, president of IUPAC take on a critical importance:

“... a rather large percentage of the population associates chemistry with issues such as environmental degradation and cancer.”

“Chemists must make sure that chemistry comes across loud and clear, and takes credit where credit is due.”

“...chemistry will be essential to solving the vexing problems facing mankind, including energy, sustainable development, health, materials and food production.”

In conclusion, I would suggest going to the website created by the American Chemical Society (<http://iyc2011.acs.org>) to view a 365 day calendar of positive contributions made by chemistry to society.

You can still go to the site and add your own favourite but quite a few, as shown below are already listed:

1. Agriculture: Fertilizers: Haber Process (N_2 to NH_3)
2. Medicinal Chemistry: Antibiotics
penicillin, aspirin, sulfonamide, ibuprofen, insulin, vitamins, taxol,
morphine, ascorbic acid, steroids (contraceptive),
genome(s)
3. Refrigerants: TFE (tetrafluoroethane) allowing the safe distribution of food.
4. Materials: aluminum, batteries, polymers (fabrics, etc.),
bakelite, synthetic rubber, carbon fibers, Teflon, AstroTurf, etc.
5. Electronics: high purity silicon for semiconductors, computers, cell phones, cameras, lcd displays, solar cells
6. Optical Fibers: high purity silicon dioxide
7. Health: pasteurization, refrigeration and frozen foods, water chlorination,
vitamin C, artificial sweeteners, diagnostic test strips, unleaded gasoline,
insect repellents (DEET)
8. Chemical Instrumentation: NMR (imaging), X-ray, lasers, pH
9. Understanding the effect of CFC's on the ozone layer.

So, finally, can we assert “Better Living through Chemistry”? In my opinion, indeed we can.

Upcoming Training Seminar/Workshops

Workshop on Science Education Outreach

A workshop on “Science Education Outreach” is being organized in academic collaboration with various scientific bodies related to science, on **13th October (Thursday)** at Adamantane House.

The aim of this workshop is to bring together personnel from all fields related to science education to express their views. Workshop recommendations would be made available to all the relevant authorities.

A nominal registration fee of Rs. 1000 will be charged from the participants. For further information and registration kindly contact Dr. Vinitha M. Thadhani (vinitha.ichemc@gmail.com)

Resource Persons:

Profs. Sunethra Athukorala & M.D.P.D Costa, Drs. Sunethra Karunartne, Jayantha Watthavidanage & Vinitha M. Thadhani, Mr. C. M. R. Anthony, Mr. M. P. Vipulasena.

Training Seminar on Nanotechnology

A Training Seminar on Nanotechnology will be held on **30th September (Friday)** at Adamantane House. The objectives of this seminar is to give the Sri Lankan society a proper understanding about nanotechnology and its applications. Principles of nanotechnology as well as its applications in different areas of sciences and industry will be discussed.

Resource Persons:

Profs. RMG Rajapakse & ADLC Perera, Drs. MNS Kottegoda, A Mahavithana, J Premaratne, AR Senanayake, V Seneviratne, RGSC Rajapakse, U S K Weliwegamage and Mr. CH Manoratne.

Industrial Photochemistry

Professor Pradeep M Jayaweera

Department of Chemistry, University of Sri Jaywardenepura, Nugegoda

Photochemistry is an experimental technique that produces chemical compounds with the help of electromagnetic radiation[1]. Often photochemists perform these reactions by the action of visible or ultraviolet radiation and these processes generally involve direct participation of an electronically excited state of a molecule.

UV				Visible			
Deep UV	UV C	UV B	UV A	Blue	Green	Yellow	Red
100-200	200-280	280-320	320-400	400			700

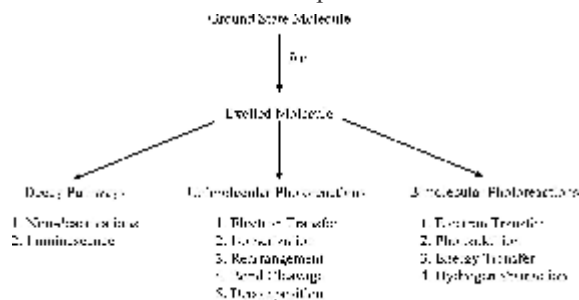
UV-Visible Spectrum (Wavelength in Nanometers)

Many life processes involve photochemical reactions, such as photosynthesis and vision[2]. This reflects the fact that the major source of energy on earth is the Sun's radiation. Like any other technique, photochemical methods have some advantages over thermal, catalytic and various other methods. These advantages include: Activation of individual reactants selectively; electronically excited states of a molecule have different reactivities; thermal load on the reaction system minimal; exact control of radiation in terms of space, time and energy. Since an electronically excited state of a molecule (M^*) has a higher internal energy than the ground state (M), there exists a much greater choice of reaction product (P) for the excited state on thermodynamic grounds. The comparison is between a reaction $M \rightarrow P$ and $M \rightarrow M^* \rightarrow P$, and for many systems $M^* \rightarrow P$ is thermodynamically favorable, where the corresponding $M \rightarrow P$ is not. In a photochemical reaction, thermal equilibrium between excited state, intermediate(s) and product(s) is rarely achieved, because of the magnitude of the energy change involved and high rate constants involved in individual steps.

Nevertheless, photochemistry is not without its own specific problems, some of them are: *Absorption characteristics* - Only absorbed light can be used for chemical purposes. Hence, many reaction systems are not suitable for photoreactions because of their unfavorable absorption characteristics. *Internal/External light filters* - Photoreactions may rapidly approach to a halt if products with competing absorptions are formed during the photoreaction. *Investment cost* - Industrial scale photochemical factories may need high unit capital costs. Limitations are imposed by the power of the lamps as main factor. *High electricity costs* - It is a fact that light is more expensive than heat, because considerable losses, as heat occur in the production of electrical energy and its conversion into usable light energy.

Therefore, when applying photochemical techniques to industry, an industrial photochemist must understand and try to bring out the full advantages of photochemistry and minimize the difficulties inherent in the method. The main aim and target of an industrial photochemist should be to reduce manufacturing costs for chemicals by introducing photochemical steps in the syntheses. Photochemical reactions have made considerable impact in synthetic chemistry, both research laboratories and in commercial processes. Light-sensitive compounds have great technical significance in photography and printing. Important applications have been also found in UV-curable paints, primers, and printing inks. Photostabilizers are primarily used in plastics and man-made fibers. Another interesting field of application is sunscreen cosmetics. In the synthesis of compounds with special spectral properties, attention is focused on lightfast dyes, optical brighteners, fluorescent dyes, and chemiluminescent systems.

The main photochemical contributions to our ecology come as chemical storage of solar energy. Investigations on the photodegradation of biologically active ingredients, photochemical smog formation and the development of photodegradable plastics are few areas where industrial application could play a major role. For all these tasks the theoretical and practical assistance of pure photochemists is extremely useful. Difficulties sometimes arise due to the fact that the photochemists at the universities are usually less concerned about commercial products.



Photochemical Pathways

The deactivation pathways of an excited molecule are shown in the above flow chart. In this article few deactivation processes have been selected and an attempt was made to understand the processes with appropriate industrial applications.

Luminescence

Luminescence[3] is the emission of light by a

molecule that is not resulting from heat; it is thus a form of cold body radiation. The process can be represented as $M^* \rightarrow M + h\nu$. There are number of different types of luminescence processes so far identified by scientists namely: Photoluminescence, Chemiluminescence, Electroluminescence, Mechanoluminescence, Thermoluminescence, Sonoluminescence etc. Let us consider few industrial applications of photoluminescence process. The most well understood two photoluminescence processes are fluorescence and phosphorescence. Optical brightening agents (OBA) or whitening agents that are used as an additive in laundry detergents uses the principle of fluorescence. The active ingredient is a dye molecule that absorbs light in the ultraviolet region and re-emits light in the blue region. Optical brightening agents are used in many other industries, such as paper industry to produce high brightness papers, as fiber/textile whitening agents and color-correcting agents. Commonly used OBAs include compounds like biphenyl-stilbenes, triazine-stilbenes, benzoxazolines.

Non-radiative (radiationless) Deactivation

The emission of light through the process of luminescence is visible to our eyes or if not to sensitive detectors. However, conversion of the electronic energy possessed by excited molecules into heat is less striking. Nevertheless, non-radiative deactivation to the ground state has a much more far-reaching significance to us than radiative deactivations. The process can be express as $M^* \rightarrow M + DH$. Objects that we use in everyday life, such as foodstuffs, paints, plastics, dyes or textiles, are changed on exposure to Sunlight and are finally destroyed. Human skin is no exception for this photodegradation process. In fact there is a saying that a woman at age forty who has protected her skin from the Sun actually has the skin of a thirty year old. Protect from Sun's radiation and to minimize the destructive effect due to nonradiative deactivation is a multi billion industry today. Research work is on at a high level to synthesize photostable and risk free compounds that are capable of converting absorbed light into heat effectively. Commonly used and FAD approved active ingredients in sunscreens include p-aminobenzoic acid, phenylbenzimidazole sulfonic acid, menthyl anthranilate etc.

Electron Transfer Reactions

The process of photo-induced electron transfer (PET) can be expressed as $M + h\nu \rightarrow M^* \rightarrow M^+ + e^-$. Photoinduced electron transfer (PET) is the branch of photochemistry that exploits the ability of certain photoexcited molecules to act as strong oxidizing or reducing species, and induce a permanent chemical change in a ground state molecule through an electron transfer mechanism. There are innumerable industrial applications of this process, photoconductors in photography, imaging systems such as silver halide

photography, solar-cells, sensors, electronics devices and photosynthesis are some few examples. The reverse of PET process is exhibited by light emitting diodes (LED).

Energy Transfer Process

The process of electronic energy transfer can be represented as $M + h\nu \rightarrow M^* + B \rightarrow M + B^*$. This photochemical principle is used in common fluorescent lamps. The basic function can be explained in the following manner: When a high potential is applied, ionization of inert gas and subsequent recombination of stray electrons produce excited atoms of the inert gas inside the tube; $Ne + e^- \rightarrow Ne^+ + 2e^-$; $Ne^+ + e^- \rightarrow Ne^*$. The energy transfer from excited Ne atoms to ground state Hg take place through collisions, resulting an emission of UV light. $Ne^* + Hg \rightarrow Hg^* + Ne$; $Hg^* \rightarrow Hg + h\nu$. Doping the lamp with rare earth compounds like Tb^{3+} , Ce^{3+} :LaPO₄, Tl etc. can produce different emission outputs lines with the energy transfer process; $Hg^* + Tl \rightarrow Hg + Tl^*$; $Tl^* \rightarrow Tl + h\nu$.

Isomerization/addition reactions

Photo-induced isomerization and addition reactions can be represented as $M^* \rightarrow X$ and $M^* + Y \rightarrow MY$ respectively. Industrial applications of these two processes are extensive. The synthesis of vitamin D3 is a very good example, where photoinduced isomerization comes in to play. When 7-dehydrocholesterol is exposed to UV-B light previtamin D3 is formed and it spontaneously isomerizes to vitamin D3. An industrial application of photo-induced addition reactions like maleic anhydride with aromatic compounds has found way to develop heat-resistant coatings.

Future of Photochemistry:

It is now widely accepted throughout the scientific community that both photochemical and photophysical processes are well understood for molecular systems. However, two areas like heterogeneous photochemical reactions on nanomaterials and sonoluminescence find much interest among scientists to find new pathways in photochemical processes that can be used as potential tools in industrial applications. Heterogeneous photochemistry on nanomaterials such as nanodust have shown size dependent redox chemistry[5] with newly identified mechanisms and reaction pathways. These newly identified photoreaction pathways in conjunction photoactive nanomaterials such as TiO₂, ZnO etc definitely have future industrial photochemical applications.

The effect of sonoluminescence involves the conversion of acoustical energy to optical energy. The effect was first discovered at the University of Cologne in 1934. Studies performed with single-bubble

sonoluminescence[6] have indicated that interior of the collapsing bubble reaches to a temperature 10,000 – 20,000 K with the core of bubble approaching to a density equal to the solid state. These exploding bubbles generally viewed as high-temperature, high-pressure, miniature reactors. Although the fusion has been ruled out, future of the process is viewed as a promising area having huge impact on industry. The more interested readers might find the BBC documentary broadcasted with the title “An Experiment to save the World”.

Reference:

1 M. Pape, Industrial Applications of Photochemistry, BASF AG, Hauptlaboratorium, 67 Ludwigshafen, GFR.

2 J. B. Thomas, Primary Photoprocesses in Biology, North_Holland, Amsterdam (1965); D. O. Cowan and R. L. Drisko, Elements of organic Photochemistry, Plenum Pres, New York (1976), Chapter 12.

3. <http://en.wikipedia.org/wiki/Luminescence>

4. <http://photochemistry.wordpress.com/tag/photoinduced-electrontransfer/page/2/>

5. Reactions on Atmospheric Dust Particles: Surface Photochemistry and Size-Dependent Nanoscale Redox Chemistry, G. Rubasinghege, S. Elzey, J. Baltrusaitis, P. M. Jayaweera, and V. H. Grassian, J. Phys. Chem. Lett. 2010, 1, 1729–1737.

6 Sonoluminescence: Inside a micro-reactor, D. Lohse, NATURE, 2002, 418, 381-382.

Photochemistry and Medicine

Dr. Ranil De Silva

Senior Lecturer, Dept of Anatomy, Faculty of Medical Sciences, University of Sri Jayewardenepura, Nugegoda

Photomedicine is the study and treatment of diseases caused by exposure to light and diagnostic and therapeutic application of light for detection and curing diseases. In the diagnostic field of photochemistry, the principles which are used are light scattering, light emission and light absorption. The diagnosis could be identified by absorption of fluorescent dyes and the tissues optical properties.

Therapeutic photomedicine categorized into phototherapy, laser therapy, photopheresis and photodynamic therapy. In phototherapy, the light energy is transformed to chemical, heat and kinetic energy to give the desired physiological reaction. Laser therapy causes local damage by selectively heating damaged matter (blood and melanin), while not heating the rest of the skin. Biomedical applications in photochemistry have been established in the fields of surgery, dentistry, ophthalmology, oncology and molecular biology and dermatology.

Effects of light on the skin include production of Vitamin D, tanning, chronic exposure include ageing (photoaging) of the skin, and the skin cancers basal cell and squamous cell carcinomas, and malignant melanoma. Harmful acute effects of sun exposure include sunburn and various photodermatoses. The interaction of UV light with the skin causes a complicated cascade of events that involve cellular damage and repair, pigmentation changes, vascular and immune suppression effects. Diagnostic uses of light include luminescence [photo and chemi] in immunoassay, fluorescence in cell sorting, and the various forms of fluorescence microscopy, including confocal, fluorescence lifetime imaging [FLIM], and single molecule. Therapies include the PUVA ("PUVA" stands for the use of a psoralen drug (P)

in combination with Ultraviolet A (UVA) light) treatment of psoriasis and vitiligo, blue light curing of neonatal jaundice, photoinactivation of microbes. Laser treatments include ablative corrective eye surgery (LASIK), general 'bloodless' surgery, and of most importance photochemically, the various treatments using sensitizers and laser light known as Photodynamic Therapy, PDT. Photodynamic therapy (PDT) is a two-step therapeutic technique in which the topical or systemic delivery of photosensitizing drugs is followed by irradiation with visible light. Activated photosensitizers transfer energy to molecular oxygen, generating reactive oxygen species (ROS). The subsequent oxidation of lipids, amino acids and proteins induces cell necrosis and apoptosis.

Sharing similar basic mechanisms of photochemistry, these applications do differ in many aspects including target molecules, molecular action, light source and optical windows.

Photochemically induced cerebral infarction model for ischemic stroke has been considered a clinically relevant model. This model is closer to a blood brain barrier (BBB) injury model than a thrombotic stroke model and may be useful to study mechanisms regulating BBB permeability.

Green tea is a popular beverage consumed worldwide. The epicatechin derivatives, which are commonly called 'polyphenols', are the active ingredients in green tea and it possess antioxidant, anti-inflammatory and anti-carcinogenic properties. Studies conducted human skin have demonstrated that green tea polyphenols (GTP) prevent ultraviolet (UV)-B-induced cyclobutane pyrimidine dimers (CPD), which are considered to be mediators of UVB-induced immune suppression and skin cancer induction.

A study conducted by us to compare *in vitro* the effects of cell viability, gene expression and the proteins levels involved in apoptosis by flavonoids from Ceylon green tea on hypoxic human brain epithelial cells (HBEC), as compared to controls, demonstrated that flavonoids from Ceylon green tea were able to reduce the amount of apoptosis after

inducing hypoxia. The expression levels of the pro-apoptotic genes were down-regulated and the expression of the anti-apoptotic gene was up-regulated resulting in higher cell viability, frequent drinking of Ceylon green tea may be neuroprotective against neurodegenerative diseases and stroke.

Photochemistry in the atmosphere

Professor K R Ranjith Mahanama

Department of Chemistry, University of Colombo.

Photochemical reactions are chemical processes that are caused or accelerated by light. Since light is a form of energy, under proper conditions it can supply energy to drive chemical reactions which would otherwise be unfavorable energetically. These photochemical reactions are of greater importance environmentally because sun can provide the necessary energy to drive such chemical processes. The most important environmental photochemical reaction is the photosynthesis. Through the photosynthesis, solar energy is harvested and stored as chemical energy by combining atmospheric carbon dioxide and water producing carbohydrates. Atmosphere is receiving oxygen as a byproduct of photosynthesis process. These products from the photosynthesis are essential for the existence of life on earth and also help to mitigate the levels of carbon dioxide in the atmosphere, thus reducing the contribution to the global warming. Photosynthesis cannot proceed in the absence of light but its reverse reaction, respiration, is spontaneous even in the absence of light. Intention of this paper is not to discuss photosynthesis in detail, but to address two existing problems namely, tropospheric photochemical smog and stratospheric ozone layer depletion.

First let us have a brief look at our atmosphere. Atmosphere is a blanket which is supposed to nurture and protect the life on earth while maintaining a thermal comfort for the existence of life. In fact it plays these three key roles and sustains the life on earth, but, anthropogenic inputs often termed as pollutants have disturbed the natural equilibrium of the atmosphere as well as the life on the earth. Though it spreads into a larger region, atmosphere is very thin, analogues to the skin of an apple and the photochemical reactions have a significant effect on the global atmospheric chemistry. Even though the pressure and the relative density of the atmosphere decrease with altitude, temperature undergoes several inversions. Based on the thermal inversions atmosphere is divided into different regions namely troposphere, stratosphere, mesosphere and thermosphere and the inversion boundaries are known as tropopause, stratopause and mesopause. Figure 1 indicates the four regions, distribution of the chemicals within them and the penetration of solar radiation into these regions. As Figure 1 indicates, the chemical nature of a substance varies from a sphere to another

sphere and this is attributed to the differences of solar radiation received.

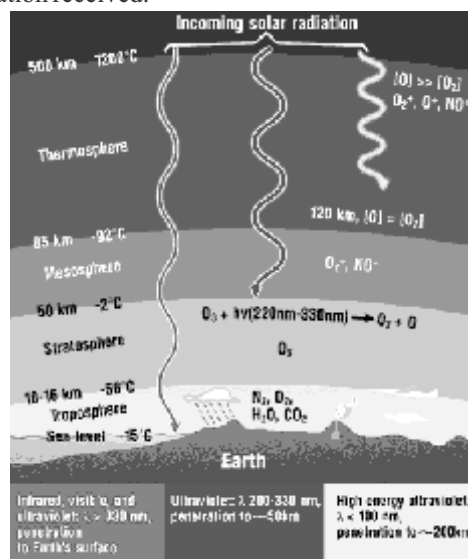


Figure1: Different regions of the atmosphere, temperature variations in these regions, penetration of solar radiation, and the existence of different forms of the chemicals in the atmosphere

Troposphere receives, IR, visible and low energy UV radiations and they do not have sufficient energy to cleave a bond or to make a chemical change. Thus the photochemical reactions are limited in the troposphere. Visible energy penetrated to troposphere may excite the molecules making them colorful while IR energy can only rotate the molecules. Stratosphere being the recipient of UV has the ability of cleaving the bonds converting molecular oxygen to ozone *vice versa*. Both mesosphere and troposphere having less mass (like a vacuum) receives high energy UV producing the ions and atoms through photochemical reactions. Though these ions and atoms are highly unstable, they survive in these two regions due to lack of other species for collisions to initiate the chemical changes. Thus the photochemistry of atmosphere varies from region to region. Furthermore, atmospheric photochemical reactions consume high energy radiation preventing their penetration to earth protecting the life on earth.

Troposphere is the technical term for the lower

atmosphere and its chemistry is dominated by the oxidation of trace atmospheric components. When the anthropogenic inputs are elevated they are getting oxidized by hydroxyl radicals forming numerous reactive intermediates and secondary pollutants which make significant health and environmental problems. One such process is known as photochemical smog. The term smog is derived by merging the two terms smoke and fog. Photochemical smog was first coined to identify the environmental disaster which took place in Los Angeles, California in 1940's. The emissions from vehicles were trapped in the zonal area of Los Angeles due to the meteorological conditions causing stagnation of airborne pollutants. The hydrocarbons and oxides of nitrogen emitted from the internal combustion engines were the imitative chemicals of the photochemical smog and they were known as primary pollutants of the LA smog. These primary pollutants were gradually converted to secondary pollutants which included oxidants such as aldehydes, ozone and peroxyacetyl nitrate (PAN). Production of these secondary pollutants with the expense of primary pollutants was driven by light and the initiations of such reactions were centered on the hydroxyl radical.

The extremely reactive hydroxyl radical exists in troposphere for less than 1 second before undergoing chemical reactions. The atmospheric levels of the hydroxyl radicals vary from zero (in dark) to 10^7 radicals in a cm^3 . The unstable hydroxyl radical gets stabilized by abstracting hydrogen from a hydrocarbon or by adding to an unsaturated centre. All these processes are energetically feasible because the resulting chemicals are stable molecule. For example, hydrogen abstraction is favored by the formation of a stable O-H bond which is stronger than a less stable C-H bond in a hydrocarbon where H is abstracted from. Through the hydrogen abstraction, relatively less reactive hydrocarbon is converted to a radical and it can initiate a series of other reactions with tropospheric gasses. These reactions yield a series of reactive intermediates and products which are threatening the health and the environment.

It is worth to look at the mechanism involve in the formation of the tropospheric hydroxyl radical. A complicated set of reactions driven by sunlight generates the hydroxyl radicals. First, nitric oxide (NO) is formed whenever air is heated. This endothermic reaction happens in internal combustion engines, glowing cigarette tips, cooking stoves or during natural activities such as thundering and lightening. Thus produced NO gets oxidized to nitrogen dioxide (NO_2) with powerful atmospheric oxidants such as ozone. Oxidation of NO by molecular oxygen (O_2) is a very slow and unproductive process. Brown NO_2 absorbs both visible and UV regions of the spectrum, however, cleaving the N-O bond occurs when the wavelength of the solar radiation is less than 400 nm. Photolysis of NO_2 produces NO and atomic

oxygen (O). The unstable O reacts quickly with O_2 forming O_3 . Photolysis of ozone yields O and O_2 which can be either in their ground states or excited states. Ground state O combines with O_2 to form ozone and O does not have sufficient energy to cleave a stable O-H bond in a water molecule. Only the excited O has sufficient energy to cleave the stable O-H bond forming two hydroxyl radicals.

Four basic conditions are necessary before the photochemical smog can develop which includes oxides of nitrogen, hydrocarbons, sunlight and temperature above 18°C . As mentioned earlier oxides of nitrogen and sunlight are required to form the important hydroxyl radicals and they attacked on the hydrocarbons to form the oxidants. Temperature above 18°C provides the necessary activation energy for the photochemical reactions. Photochemical smog is found in all the big cities which satisfy the above four requirements. Physical characteristics of the photochemical smog include a yellow-brown haze which reduces the visibility and the presence of substances not only irritates the respiratory tract but also cause eye watering.

The consequences of photochemical smog are mainly due to the toxicity of the secondary pollutants such as ozone and PAN. Respiratory impairment results from the breathing air containing more than 0.1 ppmv of ozone, especially by persons suffering from respiratory complaints such as asthma and emphysema. Although ozone and PAN are toxic to animals and people, they are much more toxics to plants. At 0.1 ppmv of ozone, the rate of photosynthesis of the plants is reduced by a factor of two. This was clearly evident in citrus farm lands in Los Angeles county and other suburban cities. Californian farmers helped the local authorities and central government financially to investigate the cause for failures in citrus farming. These investigations unraveled the chemistry behind the photochemical smog and Californians introduced the toughest regulations for vehicle emissions to abate the photochemical smog. Emission controlling devices such as catalytic converters were introduced for motor vehicles to reduce the emissions of primary pollutants. In a catalytic convertor, two different chemical processes are done on the catalyst surfaces at two different stages. In the first stage nitrogen oxides (NO_x) are reduced to nitrogen and at the second stage partially combusted organic compounds and CO are oxidized with excess air at a lower temperature to carbon dioxide and water avoiding further formation of NO_x .

Signs of photochemical smog in Colombo are visible in terms of brown haze and increasing hospitalizations due to respiratory problems. In Colombo and suburbs high vehicle density, traffic congestions, uncontrolled emissions and improper combustion conditions elevates the levels of primary

pollutants and the intense sunlight in Colombo facilitate the conversion of motor vehicle emissions to oxidants. Fortunately, air is not getting stagnated in Colombo. Indian Ocean is serving as a buffer which helps to disperse the pollutants into the sea or into the inlands. However, if the high rise buildings are erected along the coastal belt, Colombo will be an ideal location for photochemical smog threatening the health and life of the Colombo and suburb city dwellers. It is reported that the Kandy is experiencing the problems associated with the photochemical smog. It is not a wonder that the hill city with the surrounding mountain ranges experience thermal inversions leading to the stagnation and accumulation of pollutants promoting the photochemical smog.

As discussed earlier tropospheric ozone is a threat to the human life and it is known as *Bad Ozone*. However, ozone in the stratosphere prevents the penetration of UV radiation, thus protecting the life on earth earning the name of *Good Ozone*. Importance of stratospheric ozone is emphasized by the term ozone layer but it gives a wrong impression that ozone is the main constituent in the region. In fact the highest level of ozone in the region is 10 ppmv near altitude of 35 km. Thus it is a trace gas in both the spheres and if all the ozone were compressed to a single layer at STP, ozone accounts for a thickness of about 3 mm only.

In the stratosphere, under the influence of sunlight O_2 is continually being changed to O_3 and O_3 is likewise converted back to O_2 . Each day 350,000 tonnes of ozone are made and destroyed in the stratosphere. Light absorption by stratospheric O_2 and O_3 is responsible for protecting the earth's surface from radiation having $\lambda < 320$ nm. O_2 is the main absorber near 200 nm while O_3 is more important in the range of 230 -320 nm. These two natural processes of ozone formation and destruction would bring the ozone to a steady state. In addition to the two natural processes, there is evidence that ozone level has been affected by the presence of radicals in the stratosphere. These radicals have served as the catalysts in destroying the levels of ozone and the process is known as ozone layer depletion. For example single chlorine radical can destroy 20,000 ozone molecules before it is removed from the catalyzed destruction process.

Photochemical reactions are contributing factors for the production of radicals that catalyze the formation of ozone. Among the radical forming compounds, chlorofluorocarbons (CFCs) have been identified as a major contributor to the ozone layer depletion. These CFCs, once recognized as miracle chemicals, have excellent properties of chemical inertness, physiological inertness, non flammability, low surface tension, low boiling points, low viscosity, high molar enthalpy of vaporization, compressibility and expandability. Thus they were widely used as industrial chemicals in refrigeration, in aerosol formation, in foam manufacturing and as cleaning

solvents. Since CFCs were considered as non harmful chemicals with no significant impact to the environment or health, they were used without any control and they were released to the environment freely assuming no future threats.

In the troposphere, CFCs are non reactive and serve as greenhouse gases contributing to the global warming. Once CFCs were escaped to stratosphere, they are exposed to UV radiation which leads to slow photolysis of the C-Cl and C-F bonds of the CFCs creating the radicals to catalyzed the ozone destruction. Thus, photochemistry not only plays a major role in the natural formation and destruction of ozone but also in the catalytic destruction as well. Since the residence time of CFCs are in the range of 50 – 100 years, environmental damage cause by CFCs is a problem that could persist for many generations.

It is worth to discuss the contribution of photochemistry towards the reduction of ozone levels in the Polar Regions which is commonly known as *Ozone Hole*. In fact the term *Ozone Hole* is a misnomer and it implies that there is no Ozone in the region. In reality the ozone levels in the Polar Regions reduces up to 50% but it never makes the ozone level to be zero. Two important factors that contribute to the formation of the *Ozone Hole* are polar stratospheric clouds (PSCs) and vortex formation in the winter months. In dark winter months, natural formation and destruction of ozone comes to a halt and vortex isolates the region which has no air mixing from other areas, Figure 2. Thus the levels of ozone in the isolated region remain constant and there is no *Ozone Hole* or even there is no depletion of ozone in the isolated region. Thus there is no *Ozone Hole* in the winter months.

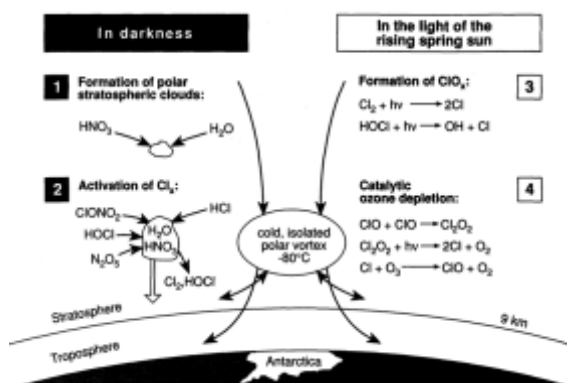


Figure 2: Chronology of the Antarctic *Ozone Hole* formation.

As illustrated in Figure 2, PSCs acts as adsorption sites for inactive forms of chlorine which will not release the chlorine radicals for the depletion. Thus chemicals such as $ClONO_2$ are deposited on the surfaces of the crystals of HNO_3 , $3H_2O$ and ice. These crystals are formed when the temperature reaches below $-70^\circ C$ and the chlorine containing chemicals such as $ClONO_2$ and HCl break down on the surfaces

of these crystals, producing Cl_2 and HOCl . These Cl_2 and HOCl formed from heterogeneous reactions on the ice surfaces are capable of photolysed by visible or low energy UV producing radicals of chlorine to catalyze the destruction of ozone. This sudden release of chlorine radicals vigorously brings the ozone levels to as low as 50% from their winter levels. Once the Polar Regions receive the normal levels of sunlight, vortex breaks down slowly allowing the mixing of chemicals from other areas and commences the natural formation and destruction of ozone recovering the *Ozone Hole*. In summary during the winter, ozone levels in the Polar Regions remain unchanged (no *Ozone Hole*) but with the beginning of the spring *Ozone Hole* appears due to sudden release of chlorine radicals and *Ozone Hole* recovers slowly with the break of the vortex and natural formation and destruction of ozone.

The Arctic *Ozone Hole* is less pronounced compared to the Antarctica *Ozone Hole*. This is due to

the slightly warmer temperatures of the Arctic with more human activities in the Northern Hemisphere than in the Southern Hemisphere. As a result, formation of the PSCs is lesser or the clouds are not cold enough to make the crystals of $\text{HNO}_3 \cdot 3\text{H}_2\text{O}$. Thus the PSCs in the Arctic do not support the accumulation of inactive chlorine chemicals onto the surfaces to produce active chlorines. Not only that the vortex does not last long in the Arctic compared to Antarctic allowing the mixing of ozone rapidly preventing the long lasting of the Arctic *Ozone Hole*.

With these two examples it is clear that the photochemical processes in the atmosphere play a significant role on our lives and perhaps we may have understood few of them only. A sound understanding of these photochemical processes is necessary to sustain our lives and the environment. Furthermore, these photochemical processes can be utilized effectively to improve the life on earth.

Photochemical Sensors

Dr. R. Senthilnithy

Senior Lecturer, South-Eastern University of Sri Lanka, Oluvil

What are Sensors?

Sensors (detectors / transducers) cover a wide category of devices that are used to monitor, measure, test and analyse data which are generated due to changes in a measured norm. An ideal sensor should have the following characteristic properties such as small size, selectivity, sensitivity and also should have the ability to communicate. There are different classes of sensors such as, temperature sensors, rate sensors, pressure sensors, magnetic sensors, position sensors, flow sensors, force/strain sensors, electro-optical sensors, acoustic/vibration sensors, acceleration sensors, biological sensors and chemical sensors.

Chemical Sensors

“A chemical sensor is a device that transforms chemical information, ranging from the concentration of a specific sample component to total composition analysis, into an analytically useful signal”. The chemical information, mentioned above, may originate from a chemical reaction of the analyte or from a physical property of the system investigated. Chemical sensors can provide real-time and on-line information on the presence of specific compounds or ions in complex samples. Usually an analyte recognition process takes place followed by the conversion of chemical information into an electrical or optical signal.

Fluorescence Sensors

Fluorescence sensing of chemical and

biochemical analytes is an ongoing active area of research. These efforts are driven by the desire to eliminate the use of radioactive tracers, which are costly to use and waste dispose problems. There is also a need for rapid and low-cost testing methods for a wide range of clinical, biochemical processes and environmental applications. During the past decades numerous methods based on high-sensitivity fluorescence detection have been introduced, including DNA sequencing and DNA fragment analysis.

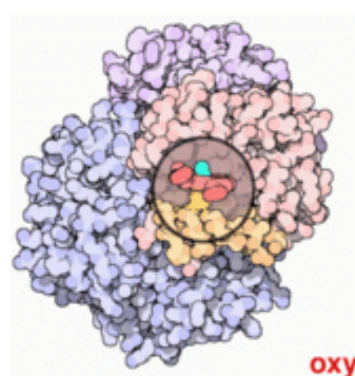


Fig. 1: Fluorescence detection on DNA fragment analysis

Fluorescence staining of gels following electrophoretic separation and a variety of fluorescence immunoassays and the **analysis of environmental pollutants** are also of current research interest.

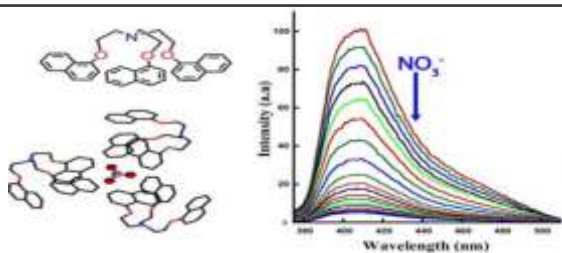


Fig. 2: Fluoremetric analysis of an environmental pollutant NO_3^- using naphthalin based tripodal ligand

Why do we need Fluorescent Sensors?

The presence or the absence of a particular material can be detected by fluorescence sensors. They have; high detection sensitivity and selectivity, 'on-off' switch ability, human-molecule communication and better space resolution ($< \text{nm}$) and time resolution ($< \text{ns-ms}$). These sensors provide a very easy communication between the system and the investigator.

Molecular structure requirements

Fluorescence is shown by those molecules which have absorbency. Some examples include;

- Compounds with multiple double bond and conjugated bonds
- Many heterocyclic and aromatic compounds.
- Metal chelates
- Compounds with certain substituted groups such as $-\text{NH}_2$ and presence of $-\text{OH}$, $-\text{OCH}_3$ on the resonating nucleus

favour Fluorescence. Electron withdrawing groups like $-\text{COOH}$, $-\text{NO}_2$, $-\text{Cl}$, $-\text{Br}$ etc diminishes or destroy fluorescence.

Structural features which affect Fluorescence

The structural features that favour fluorescence have aromatic functional groups with low $\pi \rightarrow \pi^*$ transition level, unsaturated aromatic hydrocarbons, increase ring size and degree of condensation. The structural features that diminish the fluorescence have aromatic functional groups with low $n \rightarrow \pi^*$ transition level (e.g. simple heterocyclic compounds pyridine, pyrrole and thiophene do not fluoresce), heavy atoms like halogens (decrease the efficiency due to the increasing intersystem crossing), double bond torsion, photoinduced electron transfer and weak bonds.

Advantages and disadvantages of fluorescence studies

The advantages of fluorescence method are due its sensitivity (10^{-8} mole or $1.0 \mu\text{g/ml}$) and the greater specificity than spectrophotometric method due to double choice of wavelength. The disadvantages are that the intensity depends on the pH (but in certain cases it can be an advantage also), UV light cause photo-chemical destruction, dissolved oxygen cause

quenching and all the elements or compounds are unable to exhibit fluorescence.

Mechanisms of sensing

Any phenomenon which results in a change in fluorescence intensity, wavelength ratiometry, anisotropy, lifetime and phase modulation can be used to explain the mechanism of sensing

Fluorescence intensity

The most direct sensing method measures the fluorescence intensity in response to the analyte concentration.

Wavelength ratiometry

In this application it is important to use measurements which are independent of fluorophore concentration. This can be accomplished using **wavelength - ratiometric probes**, which **display shifts** in the absorption or emission spectra **upon binding of the analyte**.

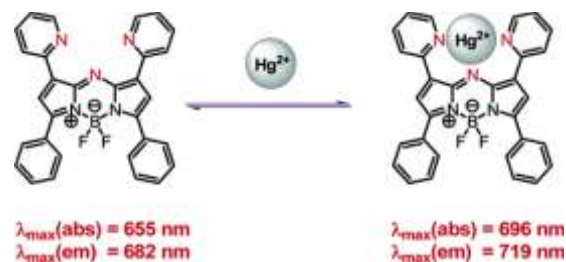


Fig. 3: Detection of Hg^{2+} using a wavelength ratiometric probe

The analyte concentration can be determined from the ratio of fluorescent intensities measured at two excitation or emission wavelengths. Wavelength-ratiometric probes are desirable because the **ratios are independent** of the probe concentration.

Fluorescence anisotropy

Anisotropy values are calculated using the ratio of polarized intensity. The use of an intensity ratio makes the anisotropy measurements independent of fluorophore concentration as long as the measurements are not distorted by autofluorescence or poor signal-to-noise ratio. Another ratiometric method is Fluorescence polarization or anisotropy. In this case the analyte causes a change in the anisotropy of the label.

Fluorescence lifetime

Fluorescence lifetimes can also be used for sensing. The lifetimes can be measured using either time-domain (TD) or frequency-domain (FD) methods. The use of lifetimes for sensing may be the next step in making sensors with long-term stability needed in real-world applications.

Fluorescence quenching

Any process which decreases the fluorescence intensity of a given substance is called quenching. This process can occur in the excited state reactions, energy transfer reactions, charge transfer reactions and complex formation reactions.

Basically, quenching process can be adopted into two kinds of mechanisms namely dynamic quenching or collisional quenching and static quenching.

Dynamic quenching occurs when the excited fluorophore contact with an atom or molecule that can facilitate non-radiative transitions to ground state. In dynamic quenching increasing the quencher concentration increases the probability of collision.

In the simplest case of collisional quenching, the following equation summarizes the fluorescence intensity and the quencher concentration and is called Stern-Volmer equation.

$$F_0/F = 1 + K_{SV}[Q]$$

Where, F_0 and F are the fluorescence intensities observed in the absence and presence of quencher respectively, $[Q]$ is the quencher concentration and K_{SV} is the Stern-Volmer quenching constant. In the simplest case, a plot of F_0/F versus $[Q]$ should yield a straight line with a slope equal to K_{SV} .

Static quenching

In some cases, the fluorophore can form a stable complex with another molecule. If the formed complex in the ground-state is non-fluorescent then it is said that the fluorophore has been statically quenched. Increasing quencher concentration increases probability of association. In such a case, the dependence of the fluorescence as a function of quencher concentration follows the equation: $F_0/F = 1 + K_a[Q]$ where, K_a is the association constant of the complex.

Förster resonance energy transfer - FRET

Any process that brings the donor and acceptor into close proximity and causes a radiation-less energy transfer will result in a decrease of fluorescence intensity and the lifetime of the donor probe is called FRET.

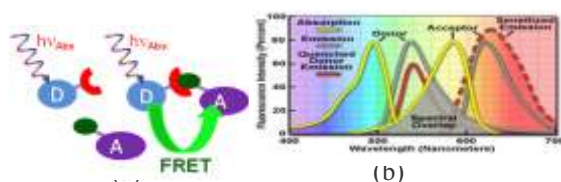


Fig. 4: (a) Schematic representation of FRET; (b) FRET donor acceptor spectral profile

This process enhances the fluorescence of the acceptor probe when the acceptor is fluorescent. Increase in fluorescence intensity of the acceptor proportional to the amount of target molecule.

Dynamic fluorescence experiments have shown that a complex has been formed between bacterial luciferase and lumazine protein. The computationally docked model of this complex has produced a separation of only 10 Å between the two fluorophores and provides evidence that shift of the bioluminescence color in the bacteria is due to FRET.

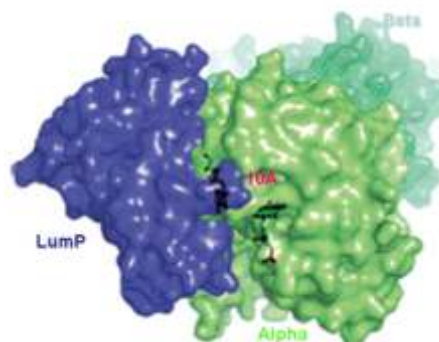


Fig. 5; Lumazine protein (LumP) associated to the alpha subunit of bacterial luciferase revealing a 10 Å separation between the lumazine binding site on LumP and the flavin-active site of luciferase.

Since energy transfer acts over a macro molecular distances, it can be used to detect association of proteins that occurs in immunoassays.

However, the applications of FRET are not limited to detection of protein association. FRET has also been used as the basis for pH and cation sensors.

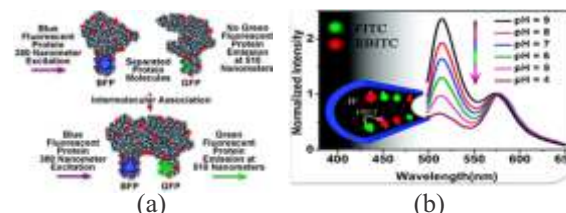


Fig. 6: (a) FRET detection of *in vivo* protein-protein interactions; (b) Schematic representation of pH sensing based on FRET

The interaction energy is of a dipole-dipole nature and depends on the distance between the molecules as well as the relative orientation of the dipoles.

Sensors have been developed that contain acceptors whose absorption spectra are dependent on the pH. A change in the pH results in a change in the absorbance of the acceptor, which in turn alters the donor intensity.

Fluorescence switch

The mechanism of fluorescence switch could be explained in such a way that when the fluorophore can exist in two forms and if the fractions of each form depend on the analyte concentration then, there is equilibrium between the fluorophore free in the solution and the fluorophore bound to the analyte. One form should be nonfluorescent, in such case emission

is seen in the absence or presence of analyte, depending on which form is fluorescent. Probes that act in this manner are not wavelength-ratiometric or lifetime probes.

In the following example protonation loses the conjugation of the system. It can absorb energy but emission may not happen. Even if it happens it may not be the same wavelength. Therefore fluorescence can be quenched or switched.

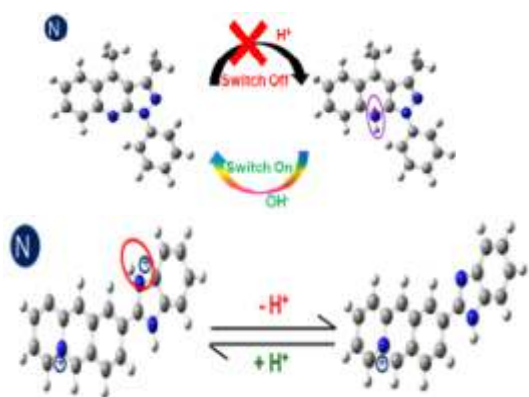


Fig. 7 : pH probes

Alternatively, both forms may be fluorescent but giving different quantum yields or emission spectra. This type of behavior is often seen for pH probes, where ionization of the probe results in distinct absorption and/or emission spectra.

Spectral shifts are also seen for probes that bind specific cations such as calcium. Such probes allow wavelength - ratiometric measurements. In this case the change in intensity or shift in the emission spectrum is used to determine the analyte concentration.

Fluorescent internal charge transfer sensors for polarity

As the polarity increases, the energy difference is lowered and emission is shifted to longer wavelengths. Sensors with emission wavelengths dependent on the polarity are useful in determining solvent polarity.

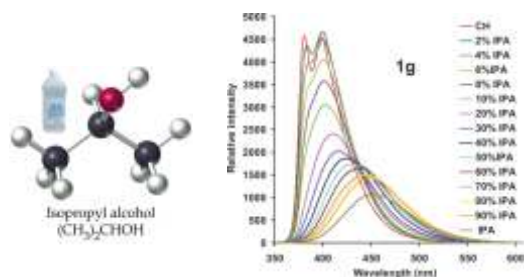


Fig. 8: Phenylethynyltriphenylenes – excited fluorescence emission spectrum in different percentage of isopropyl alcohol



Fig. 9: Fluorescent temperature sensor
With increasing temperature, about 40° C this compound gets fluorescent as green colour.

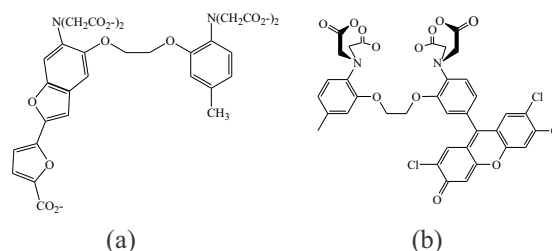


Fig. 10: (a) Ca²⁺ Sensing Integrated System; (b) Ca²⁺ Sensing Twisted System

Designing the fluorescence sensors based on Photoinduced Electron Transfer (PET)

These sensors consist of three parts, namely, fluorescence chromophore (fluorophore), receptor site and spacer between fluorophore and receptor.

A fluorophore module is the site of both photonic transactions of excitation and emission. A receptor module is responsible for guest complexation and de-complexation. A spacer module holds the fluorophore and receptor close to, but separate from each other.

There are two main types of sensors. The Fluorescence enhancing sensors in which the fluorescence is enhanced when the receptor binds to the guest and Fluorescence quenching sensors in which the fluorescence is quenched when the receptor binds to the guest.

A stimulus (analyte) changes the redox potentials of the donor – acceptor pair and will change the molecule from off state to on state.

Chelation enhanced fluorescence sensors

In this type of sensor, the fluorophore itself is non fluorescent when the receptor site is free. In the presence of metal ions the fluorescent intensity is enhanced. The 18-membered azacrown ether is highly selective for K⁺. Here the amine nitrogen requires high pH to avoid the effect of H⁺, since the protonation makes the molecule fluorescent even in the absence of K⁺.

Chelation enhanced fluorescence quenching sensors

In this type of sensor, the fluorophore itself is fluorescent when the receptor site is free. In the presence of metal ions the fluorescent intensity is lowered. In most cases the metal ion is chelated to the receptor unit of the sensor and the complex sensor is

non-fluorescent and therefore the net fluorescence is quenched.

Glucose-Sensitive Fluorophores - Glucose sensing contact lenses

The change in the boronic acid conformation from neutral to anionic form with sugar binding alters the PET mechanism of the system and thereby the fluorescence is possible.

Non-invasive continuous physiological glucose monitoring using fluorescence probes based on quinolinium backbone is a current research area leading to the development of glucose sense contact lenses.

Compound N-(boronobenzyl)-6-methylquinolinium bromide is a PET probe selective for glucose with its geometrically preferred structure. The negatively charged boronate ester form quench the fluorescence intensity in the presence of monosaccharide due to sugar complexation which is partially neutralizes the charge density at quaternary nitrogen center.

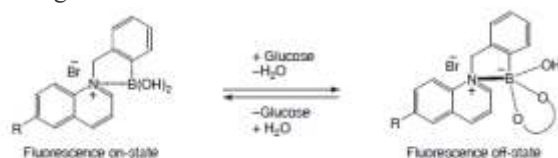


Fig. 11: Schematic representation of the charge neutralization-stabilization mechanism of N-(boronobenzyl)-6-methylquinolinium bromide with regard to glucose sensing

These new compounds with positively charged nitrogen center are highly fluorescent in aqueous solution. The charged nitrogen center is highly water soluble and thus easy to use at physiological pH.

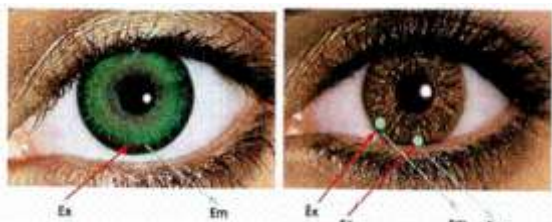


Fig. 12: The comparison of sensor spots on the surface of N-(boronobenzyl)-6-methylquinolinium bromide doped contact lens with normal eye

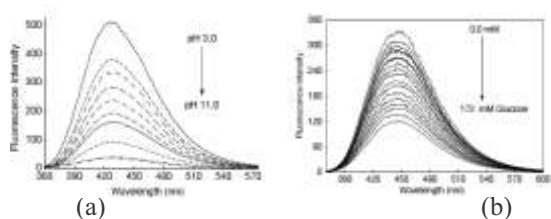


Fig. 13: (a) Emission spectra of N-(boronobenzyl)-6-methylquinolinium bromide at $\lambda_{\text{exc}} = 320$ nm in buffered media; (b) The emission spectra of N-(boronobenzyl)-6-methylquinolinium bromide doped contact lens in the presence of increasing glucose

concentrations at $\lambda_{\text{exc}} = 320$ nm.

The polymers containing N-(boronobenzyl)-6-methylquinolinium bromide are now used to prepare the contact lenses. These probes have promoted a greater understanding of the sensing mechanism and enabled the selection of the most suitable isomer based on its glucose-binding affinity.

Selective fluorescent sensor for Zn^{2+}

A new Zn^{2+} fluorescent sensor exhibits intense fluorescence after complexation with Zn^{2+} (in nano molar level) under physiological conditions. Other cations such as Na^+ , K^+ , Ca^{2+} , Mg^{2+} , Fe^{3+} , Ni^{2+} and Cr^{3+} have little influence on fluorescent enhancement for this sensor.

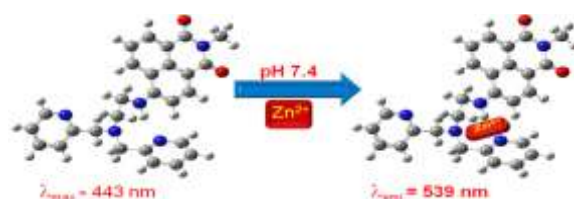


Fig. 14: Schematic representation of selective fluorescent detection for Zn^{2+}

Selective detection of magnesium ions in the presence of sodium

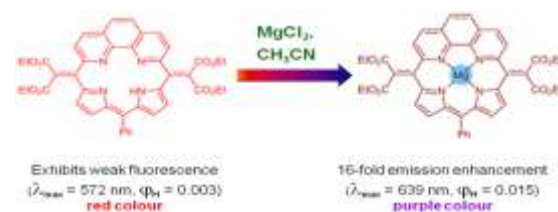


Fig. 15: Schematic representation of selective detection of magnesium ions

This porphyrin compound in the presence of magnesium ion shows emission enhancement. Sodium ion does not bind to this molecule and magnesium shows selective binding.

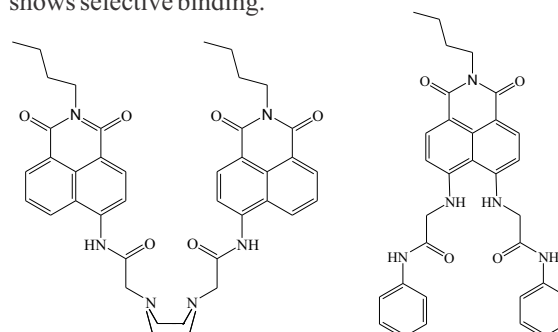


Fig. 16: Fluorescent sensor for selective detection of Cu^{2+} ions

The compounds in Fig. 16 selectively bind to Cu^{2+} and shows fluorescent enhancement.

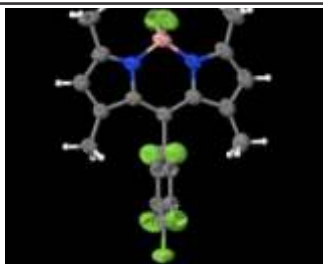


Fig. 17: 4,4-Difluoro-1,3,5,7-tetramethyl-8-pentafluorophenyl-4-bora-3a,4a-diaza-s-indacene

4,4-Difluoro-1,3,5,7-tetramethyl-8-pentafluorophenyl-4-bora-3a,4a-diaza-s-indacene is a member of a family of boron-dipyrrromethene (BODIPY) dyes. These are renowned as excellent fluorophores, exhibiting high molar extinction coefficients and high fluorescence quantum yields. They have been of recent interest with regard to the design of fluorescence labels and biomolecular sensors.

Future research on fluorescence probes should be based on the following,

- To establish flexible and portable spectroscopic devices this can be integrated in daily routine medical practice.

- To design invasive and non invasive techniques for microorganism's diagnosis inside the body cavities by use of fiber optic devices.
- Branching out of single-molecule fluorescence spectroscopy is a challenges for chemistry and influence on biology.
- Selective *in-situ* determination of analytically important cationic-anionic species.

Key References

1. Xiao Feng Zhou, *Acta Cryst.* E66, o757, 2010.
2. Ramachandram Badugu, Joseph R Lakowicz and Chris D Geddes, *Current Opinion in Biotechnology*, 16:100–107, 2005.
3. A.P. de Silva *et al.*, *Encyclopedia of Supramolecular Chemistry*, 572, DOI: 10.1081/E-ESMC 120012870, 2004
4. A.P. de Silva *et al.*, *Dekker Encyclopedia of Nanoscience and Nanotechnology*, 2749, DOI: 10.1081/E-ENN 120009336, 2004
5. M.D.P. De Costa, A.S Amarasekera and S. Perera, *Proc. Sri Lanka Association for the advancement of Science* 56(1), 228, 2000
6. A.P. de Silva *et al.* *Chem. Rev.* 97, 1515, 1997
7. M.D. P. De Costa, A. P. de Silva and S. T. Pathirana, *Journal of Canadian Chemical Society* 65, 1416, 1987.

News of Our Members

Professor J N O Fernando has been conferred the title of **Emeritus Professor** by the Open University of Sri Lanka in recognition of the contribution rendered by him to OUSL.

Professor Sudantha Liyanage has been elected as the Chairman of the Royal Society of Chemistry (Sri Lanka Section).

Mr. M R M Haniffa has been appointed as Head/Dept. of Chemistry, Open University of Sri Lanka.

Professor S Sotheeswaran attended the 5th International Congress of Chemistry & Environment in May/June in Kuala Lumpur, Malaysia. He presented a research paper on the use of Murunga (*Moringa oleifera*) Seeds in water clarification in developing countries.

Professor Sagarika Ekanayake presented a paper at the ISEKI FOOD 2011 conference held in Milan, Italy in Aug/Sept on her collaborative research with a leading food company.

(note: The travelling expenses of Profs. Sotheeswaran and Ekanayake were largely met from the Benevolent Fund of the Institute.)



Mr. Thilina Gunasekara

International Chemistry Olympiad at Tehran - Bronze Medal to CCS Student

The Sri Lankan team of two, consisted of **Thilina Gunasekara** (Final Year CCS student & third year BSc Special student of the University of Colombo) and Dilhara Jayaratna, (Final year Special student of the University of Peradeniya). Both students won bronze medals and their average put Sri Lanka at the third place while Iran and Ukraine were placed first & second respectively. Through the competition has been held since 2008, this is the first time Sri Lanka participated.

Institute of Chemistry Ceylon Fortieth Annual Sessions and Seventieth Anniversary Celebrations 2011



Chief Guest's procession



Head table of the Annual Sessions



Chief Guest:
Professor J A Pincock



Guest of Honour:
Mr. Chandima Perera



President:
Professor M P D De Costa



Main sponsor of the inauguration ceremony, Elephant House EGB handing over the cheque to Prof. M D P de Costa



Prof. Sujatha Hewage receives her Distinguished Services Award Medal



Mr. N M S Hettigedara receives his IChemC Gold Medal and prize



Ms. Anoma Wijesuriya receiving Long Service Award



Professor C. B. Dissanayake delivering the invited speech

Theme Seminar: Photochemistry for the Wellbeing of Society

held at Sri Lanka Foundation Institute, Colombo 07 on June 17, 2011

sponsored by



Iodine in the marine environment and its chemistry in the troposphere

Dr. R Parthipan

College of Chemical Sciences, Institute of Chemistry Ceylon

Iodine sources and biogeochemical cycling in seawater

Elemental iodine was first recognised in the early nineteenth century by Courtois from analysis of kelp ashes. Riley (1965) presented a review on the history of iodine measurements in the marine environment. His review identified that Pfaff made the first detection of iodine in Baltic Sea water in 1825. Iodine is the most abundant biophilic, i.e. associated with living systems and minor elements in the oceans. Its redox sensitive nature, and participation in both inorganic and biologically mediated redox reactions, makes it an interesting candidate for speciation studies. The oceans are the major natural source of iodine to the atmosphere and therefore play a vital role in determining the cycling of the element via its interactions with the atmosphere.

Iodine speciation and quantification in seawater has revealed that the most abundant species are iodate (IO_3^-) and iodide (I^-) at a total concentration of $0.45 \mu\text{mol dm}^{-3}$. Minor concentrations of dissolved organic iodine (RI) are also reported. Depth profile studies of IO_3^- , the thermodynamically stable form of iodine in seawater, generally indicate a surface minimum and increment with depth, however I^- is found in higher quantities in the surface waters and decreases with depth.

In surface waters, iodate appears to undergo reduction to iodide, which persists to depths of a few hundred meters. Recent research findings suggest certain cultures of marine phytoplankton possess the ability to convert IO_3^- to I^- .

The above findings indicate an incomplete understanding of iodine disproportionation in seawater and potential volatile sources of iodine. Iodine dynamics in seawater remains a complex picture of both biotic and abiotic activity. The natural abundance of iodine species in surface seawater are summarised in table 1.

Table 1: Iodine species and their concentrations in surface seawater

Species	Concentration/ $\mu\text{mol dm}^{-3}$
Iodate (IO_3^-)	0.1-0.45
Iodide (I^-)	0.01-0.3
Volatile organic iodine (VOI)	<0.001
Non-volatile organic iodine (NVOI)	>0.1

The inorganic chemical cycling of iodine in the ocean is primarily based on the iodide and iodate

content. The process is thought to be mediated by marine biota. Some marine algal species are capable of converting IO_3^- to I^- , indicating a complex cycling of iodine in seawater. The conversion was observed to be correlated to the specific species of marine algae. They also found that the cold water diatom *Nitzschia sp.* exhibited the highest rates ($6.84 \times 10^{-6} \text{ nmol day}^{-1} \text{ cell}^{-1}$) of iodate depletion and iodide production ($8.6 \times 10^{-6} \text{ nmol day}^{-1} \text{ cell}^{-1}$) among the three species which were observed to be able to convert IO_3^- to I^- .

This study suggests that the surface maximum of $[\text{I}^-]$ observed in seawater is not merely biologically controlled, as the limitation of such algal species to a specific location of the ocean is not sufficient to explain the wide range of observations of $[\text{I}^-]$ and therefore involvement of abiotic processes.

Various analyses have clearly demonstrated that a number of minor elements (e.g. iodine) may exist in different forms in seawater ranging in size from free ions (I^- , IO_3^-) inorganic and organic complexes, element bound to high molecular weight organic material (dissolved organic iodine), colloids, and sorbed on colloids. Within these size classes, an element may exist in different oxidation states (for iodine from -1 to +V) or protonated states. Both biological and abiotic processes have been proposed for controlling the speciation of minor elements.

Winchester and Duce (1965) reported high iodine content in seasalt aerosols, approximately 100 times greater than seawater as deduced from iodine/chlorine (I/Cl) ratios between bulk seawater and aerosols. Similar studies showed comparable results and suggested a route of iodine transfer from seawater to the marine atmosphere. Importantly, the ratio of iodine to chlorine is much higher in the air masses of marine origin than in those of continental origin. Iodine enrichment in marine atmosphere has also been reported in terms of I/Na ratios which further supported the above findings. The iodine enrichment factor calculations based on I/Na ratios are more reliable compared to those based on the I/Cl ratio because $[\text{Na}^+]$ is much more stable than $[\text{Cl}^-]$.

These observations suggest that oceans, which cover 2/3 of the Earth's surface, are the major source of iodine to the atmosphere. The iodine input from the oceans is believed to occur in the form of organically bound iodine (RI) and as I_2 . Macro algae are apparently the dominant source of both RI and I_2 in the coastal oceans while micro algae (phytoplankton) are found to be responsible for RI, predominantly methyl iodide, in the open oceans. In summary, iodine is an

important minor element present in the oceans, undergoes an array of chemical processes within the seawater, and the more volatile forms are transferred to the atmosphere. These virtues of iodine call for a comprehensive understanding of its dynamics in the seawater and in the troposphere.

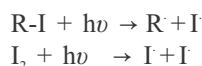
An overall picture of aqueous phase iodine chemistry in seawater along with probable abiotic mechanisms of organic iodine and molecular iodine (I_2) production is described in figure 1. RI_x stands for volatile and non volatile poly-iodinated compounds. Dissolved organic matter is indicated by DOM.

Impacts of iodine on troposphere chemistry and detection of reactive iodine in the marine atmosphere

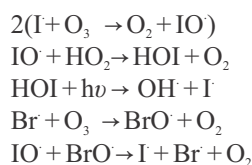
Tropospheric ozone is an important absorber in the infrared region of the planetary radiation and therefore it is also a greenhouse gas. The burning of fossil fuels over the last 2 centuries has also lead to globally increasing levels of ozone in the troposphere. This underlines the necessity for a thorough understanding of the impacts of reactive halogens on troposphere ozone chemistry.

Understanding of the exact impact of iodine photochemistry in the marine boundary layer (MBL) is still semi-quantitative due to a number of uncertainties in the sources and sinks and recycling of iodine. However, it is known that iodine is involved in the catalytic destruction of ground level ozone and the formation of aerosol precursors, also known as new particles. It is widely accepted now that the iodine new particle formation is linked to O_3 in the marine boundary layer. New particles were observed when ozone was in contact with the Laminaria surface. From this it was inferred that particles were formed by the reaction between ozone and biological iodine.

The relatively short life times of iodine vectors such as iodocarbons and I_2 from seawater rapidly produce iodine radicals which are very reactive in nature, undergo reaction predominantly with ozone, and cause a net depletion of ozone. Bromine radicals are also intimately involved in the iodine-ozone reaction cycles. These phenomena are illustrated by schemes 1 and 2, respectively.



Scheme 1: Formation of I radicals.



Net reaction

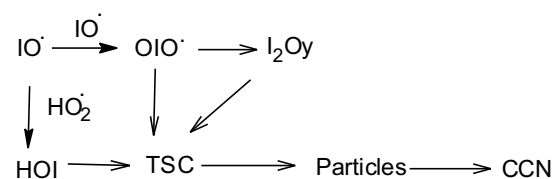


Scheme 2: Catalytic net ozone destruction cycle

involving I.

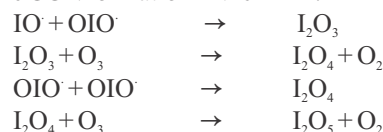
The IO radicals discussed are thought to contribute to thermodynamically stable clusters (TSC) of iodine oxides and consequent production of cloud condensation nuclei (CCN). Scheme 3 illustrates the process.

Generation of nanometre scale particles can lead to enhanced scattering of incoming radiation and net cooling of the atmosphere. To have a significant influence on climate, it would have to be effective over the oceans as a whole, not just in the coastal environment.



Scheme 3: Schematic description of formation of TSCs from IO radicals and HOI , consequent production of particles and CCN ($y=2-5$).

The initial particles produced from reactions of iodine radicals and O_3 were found to be pure I_2O_5 in laboratory studies. Reaction scheme 4 illustrates the probable production pathway for I_2O_y , where y can be 2, 3, 4 or 5. Recent quantum mechanical studies suggest I_2O_3 and I_2O_5 as stable species that would last long enough to result in new particle formation. Some chamber studies indicate that this process is viable especially during low tide events at coastal sea areas like Mace Head, Ireland. The initial TSCs are thought to grow in size and finally result in CCN which further grow to produce clouds. The exact impact of these iodine particles is a subject of ongoing research, whilst many factors such as the presence of dimethyl sulfide and its oxidation products (sulfuric acid) are also known to determine CCN formation in the MBL.



Scheme 4: Reactions leading to production of I_2O_y species.

The first successful detection of IO in the marine boundary layer (MBL) was reported in 1999 at Mace Head, Ireland. Table 2 lists the details of various field observations of reactive halogen species (RHS) in the atmosphere, using differential optical absorption spectroscopy (DOAS), an instrument based on Beer-Lambert's absorption law at different locations of the world. It is worth noting that, I_2 concentrations, even though rarely observed, are much higher than RI concentrations in the coastal MBL. While the photolytic life time of I_2 is estimated as ~ 10 seconds, the lifetimes of other iodo-carbons (CH_3I , CH_2ClI , CH_2I_2) range from days to minutes.

Table 2: Observation of iodine containing RHS in the troposphere by the active and passive DOAS technique.

Species	Location and year	Max mixing ratio./ppt
IO	Mace Head, 1997	6.7
IO	Mace Head, 1998	7.2
IO	Mace Head, 2002	7
IO	Tasmania, 1999	2.2
IO	Tenerife, Can. Islands, 1997	3.5
IO	North Sea, Germany, 2002	2.1
IO	Atlantic Coast, France, 2003	7.7
IO	Dead Sea, Israel, 2000	10
IO	Antarctic and Arctic	10
IO	Alert, Arctic, 2000	0.73
IO	Mace Head, Ireland	7
IO	Isles of Shoals, Bay of Maine	7
OIO	Mace Head, Ireland	1-11
OIO	Cape Grim, Tasmania, 1999)	3.0
OIO	Mace Head, Ireland, 1998)	9.2
OIO	Mace Head, Ireland, 2002	3.0
OIO	Isles of Shoals, Bay of Maine	25
I ₂	Mace Head, Ireland, 2002	93
I ₂	Mace Head, Ireland, 1998	61.3
I ₂	Mace Head, Ireland	93 (Night time), 25 (Day time)
I ₂	Isles of Shoals, Bay of Maine	>10 (Day time)

Summary

Iodine clearly plays various important roles in the chemistry of the troposphere. Iodine related new particle formation has a potential impact on radiative forcing (net sun radiation reaching the Earth). Based on the numerous studies carried out on iodine enrichment in the MBL from coastal seawater, it is evident that biotic mechanisms are important for iodine production and release in seawater.

The vast open ocean remains more or less unexplored in the context of the source strength of iodine. In particular, there has been little work on the contribution of abiotic mechanisms, both photochemical and thermo-chemical reactions, which have the potential to operate across the world's oceans.

Key References

- (1) Alicke, B., Hebestreit, K., Stutz, J., Platt, U., Iodine oxide in the Marine Boundary Layer, *Nature*, 397, 572-573, **1999**.
- (2) Carpenter, L. J., Iodine in the marine boundary layer, *Chem. Rev.*, 103, 4953-4962, **2003**.
- (3) O'Dowd, C., Jimenez, J. L., Bahreini, R., Flagan, R. C., Seinfeld, J. H., Hameri, K., Pirjola, L., Kulmala, M., Jennings, S. G., Hoffmann, T., Marine aerosol formation from biogenic iodine emissions, *Nature*, 417, 632-636, **2002**.
- (4) Riely, J. P., Skirrow, G., Eds., *Academic Press*, Orlando, FL, 1, **1965**.
- (5) Winchester, J. W., Duce, R. A., Geochemistry of iodine bromine and chlorine in the air-sea-sediment system, *Symposium on marine Geochemistry*, University of Rhode island, Occasional Publication, No.3, 185-202, **1965**.

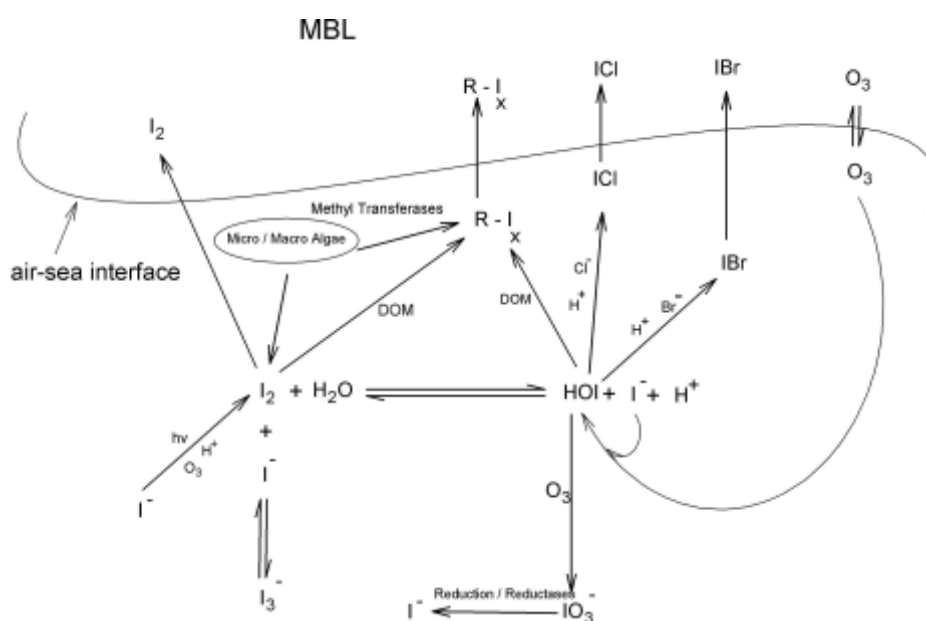


Figure 1: Chemistry of iodine in seawater and its transfer routes to the atmosphere

Nuclear Magnetic Resonance spectroscopy and *Parahydrogen*

Dr Rathika Kandiah

College of Chemical Sciences, Institute of Chemistry Ceylon

Nuclear magnetic resonance spectroscopy is a powerful diagnostic tool, used extensively to investigate the structure and interactions within and between molecules. The basic phenomenon of NMR was discovered in 1945; the spin energy levels of atomic nuclei are split by a magnetic field. Transitions between these energy levels can be induced by exciting the sample with electromagnetic radiation, which has a frequency equivalent to the energy difference between the levels. Since 1960, the field of NMR has seen an explosive growth, which started with the development of pulsed fourier-transform NMR and multidimensional NMR spectroscopy, and still continues today.

The limitations of NMR spectroscopy result from the low inherent sensitivity of the technique as well as from the high complexity and large information content of NMR spectra. These problems are partially alleviated by new developments: the sensitivity and resolution of NMR have been increased by progress in spectrometer technology. Progress in the theoretical and practical capabilities of NMR have led to the increasingly efficient utilisation of the information content of NMR spectra.

One way of overcoming the low inherent sensitivity of NMR technique was postulated in 1986 by Bowers and Weitekamp. They proposed that enhanced NMR signals could be obtained from ^1H nuclei in a product formed from the addition of molecular H_2 enriched in the *para* spin state. This technique was initially referred as *p-H₂* and the synthesis allowed dramatically enhanced nuclear alignment (PASADENA), and subsequently termed *p-H₂* induced polarisation (PHIP). The development of this technique constitutes the major part of the work presented in this article.

Theory of NMR

The basic theory of magnetic resonance results from the interaction of the magnetic moment of an atomic nucleus (m) with an external magnetic field (B_0). Most atomic nuclei have a nuclear spin (I) and that can take values 0, $\frac{1}{2}$, ...etc. In the presence of an applied magnetic field, the nuclei can orient themselves in $2I+1$ possible ways. When $I = \pm\frac{1}{2}$, these nuclei, take up one of only two orientations: a low-energy orientation aligned with the applied magnetic field, or a high-energy orientation opposed to the applied field. This difference in energy is defined by Equation 1.

Equation 1 $E = \hbar g B_0 / 2p$

Where $\hbar$ is Planck's constant, g is the magnetogyric ratio (a characteristic constant for each type of nucleus) and

B_0 is the strength of the applied magnetic field.

Where the size of the NMR signal produced from a sample molecule, and therefore the sensitivity of NMR, depends on the population difference between these spin states, the larger the difference, the larger the signal. The normal population difference depends on the Boltzmann distribution and is generally very small (because of the low-energy difference between states). The Boltzmann distribution is given in Equation 2.

Equation 2 $N_a/N_b = e^{-\Delta E/kT} = 1 - g\hbar B_0 / 2pkT$

Where $\hbar$ is the Planck's constant, g is the magnetogyric ratio, B_0 is the strength of the applied magnetic field, k is the Boltzmann constant and T is absolute temperature. This means that for a ^1H nucleus at a field of 11.7 T (corresponding to proton Larmour frequency of 500 MHz) and a temperature of 298 K, the population difference can be calculated as:

$$\begin{aligned} N_a/N_b &= 1 - [(h/2\pi k)(2.67510^8 \cdot 11.7/298)] \\ &= 1 - 8.0210^{-5} \\ &= 0.9999 \end{aligned}$$

The ratio of 0.9999 indicates that effectively only 1 in 20,000 of the nuclei will be detected in at a 500 MHz magnet. This calculation illustrates the inherent insensitivity of the technique. The technique of *p-H₂* Induced Polarisation (PHIP) typically accesses a non-Boltzmann spin distribution for the hydride nuclei attached to a metal centre. This is achieved by adding H_2 with a non-Boltzmann distribution of spin states to the metal centre.

Description of *orthohydrogen* and *parahydrogen*

Orthohydrogen (*o-H₂*) and *parahydrogen* (*p-H₂*), are two forms of molecular H_2 , and are associated with the early history of quantum mechanics. The chemical properties of the two forms are almost identical, however, they differ in their relative adsorption properties, heat capacities and electrical conductivities. It has been demonstrated that *o-H₂* is more strongly adsorbed than *p-H₂* when physically adsorbed on charcoals or TiO_2 .

The statistical ratio of *ortho* to *para* isomers was experimentally found to be 3:1 at room temperature. Statistical treatments could be applied to rationalise the proportion of the two forms with varying temperature.

Raman spectroscopy was one early technique that revealed the presence of *ortho* and *para* isomers of H_2 , which shows altering line intensities in the ratio of 3:1.

The existence of *ortho* and *para* isomers of H_2 derives from the Pauli principle, which requires that

the overall wavefunctions of fermions (protons) must be antisymmetric with respect to the exchange of nuclei.

According to the Born-Oppenheimer approximation, the overall wave function of a particle can be factorised into nuclear and electronic components. The nuclear wave function can be further divided into translational, vibrational, rotational and spin components, as shown in Equation 3.

Equation 3

$$Y = Y_{\text{electronic}} Y_{\text{nuclear}} = Y_{\text{electronic}} Y_{\text{translational}} Y_{\text{vibrational}} Y_{\text{rotational}} Y_{\text{spin}}$$

The translational function is always symmetric for the homonuclear diatomic molecule (H_2), in its ground electronic state, so are the electronic and vibrational components. Therefore it follows, that the product of the rotational and nuclear spin wavefunctions has to be antisymmetric; in order to fulfil this requirement the antisymmetric rotational states, $J = 1, 3, 5$ etc (odd values), are restricted to symmetric nuclear spin wave functions, and symmetric rotational states, $J = 2, 4, 6$ etc (even values), are restricted to antisymmetric nuclear spin wave functions. This is summarised in Table 1. H_2 molecules with symmetric nuclear spin configurations are called $o\text{-}H_2$ and those with antisymmetric nuclear spin configurations are called $p\text{-}H_2$.

Table 1 Rotational energy levels and associated spin states for molecular H_2 .

J	Rotational state	Spin state	Label
3	Antisymmetric	Symmetric	Ortho
2	Symmetric	Antisymmetric	Para
1	Antisymmetric	Symmetric	Ortho
0	Symmetric	Antisymmetric	Para

The nuclear spin wave function is characterised by magnetic quantum number, $m_i = \pm 1/2$, and it can be represented by the labels a or b , for values of $m_i = +1/2$ or $-1/2$ respectively that a particular nucleus may take. Molecular H_2 consists of two protons (x and y in this example), therefore four combinations of nuclear spin wave functions are possible, as shown:

$$Y = a_x a_y$$

$$Y = b_x a_y$$

$$Y = a_x b_y$$

$$Y = b_x b_y$$

The exchange of two identical particles cannot be detected experimentally (according to quantum mechanics). Such a process can be represented by the interchange of labels in the above example. Because altering the labels has no physical significance, the resulting states must be indistinguishable from the

initial state. Therefore, ba and ab wavefunctions are not allowed since the interchange of labels would result in a product that is different from initial state. Consequently, linear combinations of the two states must be used, termed $ab + ba$ and $ab - ba$. This is allowed by quantum mechanics, and the states are isoenergetic outside a magnetic field.

The aa , bb and $ab + ba$ wave functions are symmetric (corresponding to $o\text{-}H_2$) with respect to exchange of nuclei, whilst the $ab - ba$ state is antisymmetric (corresponding to $p\text{-}H_2$). This antisymmetric property can be explained as follows:

$$Y_{\text{spin}} = ab - ba$$

Exchange the nuclei x and y

$$Y_{\text{spin}} = ba - ab$$

$$= -ab + ba$$

$$= -(ab - ba)$$

$$= -Y_{\text{spin}}$$

It can therefore be concluded that $o\text{-}H_2$ is nuclear triplet and $p\text{-}H_2$ is the nuclear singlet. This is represented simply in Figure 1.

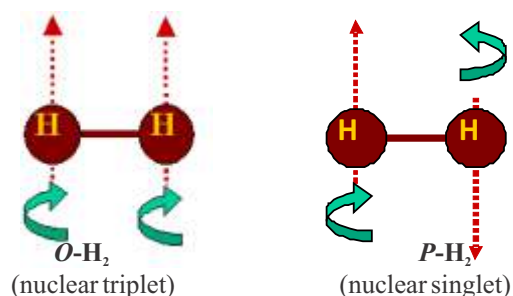


Figure 1: Spin isomers of molecular H_2 .

$P\text{-}H_2$ is more stable than $o\text{-}H_2$, as it can access a lower rotational energy state. Consequently, the difference in energies between the two isomers leads to a temperature dependent population, as illustrated in the Table 2. However, as the energy difference is low at ambient temperature, each of the four spin states is equally populated, giving rise to a 3 to 1 ratio of the *ortho* and *para* forms (as observed by Raman spectroscopy). The effect of the energy difference on the population becomes more dramatic as the temperature is reduced. The lowest rotational energy state corresponds to the *para* isomer and therefore the population of the $p\text{-}H_2$ increases as the temperature decreased.

Table 2 The effect of temperature on the relative populations of $o\text{-}H_2$ and $p\text{-}H_2$.

Temperature (K)	$o\text{-}H_2$	$p\text{-}H_2$
0	0.000	1.000
20	0.000	1.000
40	0.000	1.000
60	0.000	1.000
80	0.000	1.000
100	0.000	1.000

However, isomer interconversion requires changing a J value, and at least one value of m_l . The process is therefore forbidden. Literature indicates that the interconversion between these two isomers (*ortho* and *para*) requires of the order of a year at ambient temperature and a pressure of 1 atm. Bonhoeffer and Hartect achieved the conversion of *o*-H₂ to *p*-H₂ when passing H₂ over charcoal (a *paramagnetic* catalyst) at low temperature (78 K). This method provides a way of generating equilibrium amounts of *o*-H₂ and *p*-H₂.

Duckett *et al.* found that the >99.8% *p*-H₂ can be generated, if the H₂ gas is cooled in the presence of a *paramagnetic* catalyst using the very low temperatures that can be accessed by a closed cycle helium cooler. It should be noted that if H₂ is enriched in the *para* form, it can be brought back up to room temperature and the same proportion of the *para* form retained, as long it has been removed from the *paramagnetic* catalyst (because the interconversion back to *ortho* form cannot occur in the absence of catalyst).

The effect of *p*-H₂ on NMR spectroscopic measurements

P-H₂ itself cannot be detected by NMR spectroscopy, as it has no magnetic moment (no net nuclear spin). In order to observe a signal for *p*-H₂, the symmetry of the *p*-H₂ molecule has to be broken, therefore the two ¹H nuclei must become magnetically distinct (it is the *o*-H₂ which is seen at approximately 4.55, when H₂ is placed in a magnetic field). Breaking the symmetry of this molecule can be accomplished by a chemical reaction. Consequently, when *p*-H₂ reacts with other molecules, transferring the two protons into magnetically inequivalent positions, a signal enhancement is seen in the ¹H NMR spectrum (this is where the *p*-H₂ plays an important role in NMR spectroscopy). The effect of *p*-H₂ on the NMR spectrum (origin of enhancement) is explained using the population model for an AX spin system in the section below.

AX spin system

The AX spin system can be achieved in a simple dihydride complex with two chemically distinct but weakly coupled nuclei, far apart in chemical shift in a strong magnetic field.

The protons of the MH₂ unit will have four available spin states (spin states have to be considered together as the nuclei are coupled), which are represented by the labels *aa*, *bb*, *ab* and *ba*. In a magnetic field, these states have different energies and transitions can occur between them. NMR observable transitions only occur where the spin of one nucleus changes. As a result four transitions (*aa* → *ab*, *aa* → *ba*, *ab* → *bb*, *ba* → *bb*) can be detected by NMR and so the resultant NMR spectrum appears as a pair of

doublets.

If the MH₂ product is formed by the addition of normal-H₂ (*ortho* enriched H₂) then the energy levels will be filled according to the Boltzmann distribution (almost equally populated). Consequently, there will be a very small population difference between the energy levels; this is what permits the detection of normal ¹H NMR signals (Figure 2a).

If the MH₂ is formed by the addition of *p*-H₂, (*ab* - *ba* spin state) the product hydrides selectively populate the *ab* and *ba* states of the product, resulting in a non-Boltzmann spin distribution. This means that the population difference, and hence the intensity of the NMR signal, is much higher than the Boltzmann distribution would predict as there is potentially no population in the *aa* and *bb* spin states. This is illustrated in Figure 2b. It is worth noting that two of the transitions now occur in the opposite direction (sense), resulting in an emission absorption doublet in the ¹H NMR spectrum (the two components are antiphase to each other). This effect was observed for a reaction occurring in a strong magnetic field and named as PASADENA.

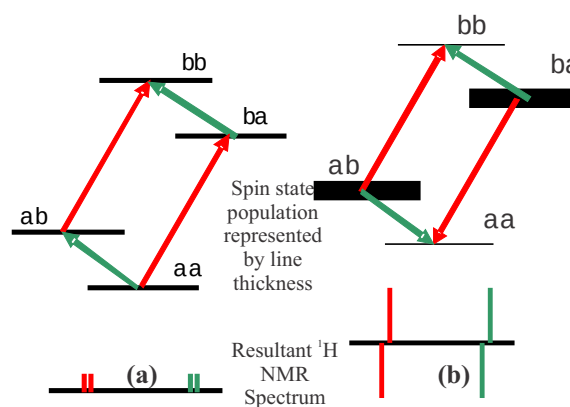


Figure 2 The distribution of spin states in (a) normal and (b) *p*-H₂ schematic representation of the corresponding peaks in a ¹H NMR spectrum for an AX spin system.

Therefore, when normal-H₂ is added to a metal complex the resulting spin states have very similar populations (Boltzmann distribution), however, if *p*-H₂ is added two of the spin states of the complex are selectively populated, resulting in a non-Boltzmann distribution and thus enhanced signal. This sensitivity gain can then be used to record information about the ligand sphere of the metal.

It should be noted that the non-Boltzmann distribution of spins must be preserved on H₂ addition in order to see the *p*-H₂ effect in the resultant NMR spectra. This means that the addition must be pair wise (so that the spin properties of the *p*-H₂ nuclei are retained) as well as rapid, relative to proton relaxation. Furthermore, the symmetry of the *p*-H₂ molecule must be broken during the addition process (hydrides have

to be distinct). If the hydrides are equivalent, it is expected that the $ab - ba$ spin state in the A_2 product spin system would be populated, and this populated spin state cannot interact with the magnetic field, resulting in no observable NMR signal. It has been observed by Aime *et al.* however, that polarisation can be transferred into the A_2 spin system, if it is formed rapidly by $p\text{-H}_2$ via an intermediate species with in equivalent hydrides.

Duckett *et al.* demonstrated that another class of spin system, where the hydrides are magnetically equivalent but chemically inequivalent, could give enhancement to a certain extent, such as in the minor product of oxidative addition of H_2 to Vaska's complex. This minor product is shown in Figure 3. The phosphorus nucleus is 100 % naturally abundant and possesses a magnetically active with spin $\frac{1}{2}$. Each of the two hydride ligand will couple to a different extent to $^x\text{PPh}_3$ and $^y\text{PPh}_3$, therefore this is an $AA'XX'$ spin system. The spin state generated on forming this species by addition of $p\text{-H}_2$ allows the observation of enhanced emission and absorption components within the resulting multiplets.

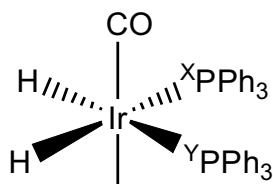


Figure 3: The minor isomer of oxidation addition of H_2 to Vaska's complex, detected by Duckett *et al.*

Moreover, a system must rapidly exchange with free $p\text{-H}_2$ in order to produce continuous enhancement. Normally, this can be achieved by heating the system. However, increasing the rate of exchange also increases the rate of $p\text{-H}_2$ consumption. In some systems, lowering the concentration of the sample can

decrease the rate of $p\text{-H}_2$ consumption. Because of these reasons, determining the optimum sample concentration and temperature are important for $p\text{-H}_2$ NMR experiments.

$p\text{-H}_2$ has been applied in many fields such as catalysis, metal hydrides, quantum computing and biomedical applications (MRI). Duckett *et al.* and Bargon *et al.* published comprehensive review articles of the chemical applications of $p\text{-H}_2$.

Key References

- 1) Sanders, J. K. M.; Hunter, B. K. *Modern NMR Spectroscopy; a guide for chemists*, Oxford University Press, Oxford, **1994**.
- 2) Bowers, C. R.; Weitekamp, D. P. *Phys. Rev. Lett.* **1986**, *57*, 2645.
- 3) Bowers, C. R.; Weitekamp, D. P. *J. Am. Chem. Soc.* **1987**, *109*, 5541.
- 4) Chapovsky, P. L.; Hermans, L. J. F. *Annu. Rev. Phys. Chem.* **1999**, *50*, 315.
- 5) Blazina, D.; Duckett, S. B.; Halstead, T. K.; Kozak, C. M.; Taylor, R. J. K.; Anwar, M. S.; Jones, J. A.; Carteret, H. A. *Magn. Reson. Chem.* **2005**, *43*, 200.
- 6) Aime, S.; Gobetto, R.; Canet, D. *J. Am. Chem. Soc.* **1998**, *120*, 6770.
- 7) Duckett, S. B.; Mawby, R. J.; Partridge, M. G. *J. Chem. Soc. Chem. Commun.* **1996**, 383.
- 8) Duckett, S. B.; Sleight, C. J. *Prog. Nucl. Magn. Reson. Spectrosc.* **1999**, *34*, 71.
- 9) Bonhoeffer, K. F.; Hartect, P. Z. *Phys. Chem. B* **1929**, *4*, 113.
- 10) Blazina, D.; Duckett, S. B. *Eur. J. Inorg. Chem.* **2003**, 2901.
- 11) Blazina, D.; Duckett, S. B.; Dunne, J. P.; Godard, C. *Dalton. Trans.* **2004**, 2601.
- 12) Natterer, J.; Bargon, J. *Prog. Nucl. Magn. Reson. Spectrosc.* **1997**, *31*, 293.

Molecular Materials: Processable Forms of Polycyclic Aromatic Hydrocarbons (PAHs)

Dr. Buddhie S. Lankage

College of Chemical Sciences, Institute of Chemistry Ceylon

Graphenes

Graphene is a one-atom-thick planar sheet of sp^2 -bonded carbon atoms that are densely packed in a honeycomb crystal lattice (Figure 1 (a)). The carbon-carbon bond length in graphene is about 0.142 nm. Graphene sheets stack to form graphite with an interplanar spacing of 0.335 nm. Graphene is the basic structural element of some carbon allotropes including graphite (d), charcoal, carbon nanotubes (c) and fullerenes (b) (Figure 1).^[1] These distinctly different types of graphitic forms exhibit unique properties which have fascinated the scientific community over the last two decades. Their unique molecular structures and the resulting extraordinary electronic, thermal and

mechanical properties make them promising candidates for future electronics and composite materials.^[2]

Polycyclic Aromatic Hydrocarbons (PAHs)

The family of flat polycyclic aromatic hydrocarbons is considered as indefinitely large aromatic molecules. PAHs such as anthracene (a), phenanthrene (b), pyrene (c), anthanthrene (d), coronene (e) etc. are widely found in domestic fossil fuels such as coal, oil, wood as well as other organic source materials (Figure 2).

All the PAHs cannot be considered as graphenes. This is because of the vast improvements in the synthesis of these large aromatic benzenoid

molecules it is now possible to substitute one or more of the ring carbons for a heteroatom such as sulphur or nitrogen. This allows the production of PAHs with heterocyclic aromatic rings (i.e. pyridine, pyrimidine, pyrrole). Through various addition reactions it is also possible to functionalise the rings themselves with various R-moities such as alkyl and alkoxy groups thereby offering various types of PAHs.

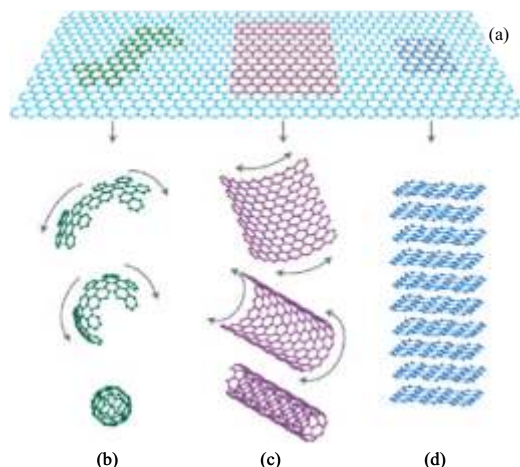


Figure 1: Graphene: the parent of all graphitic forms.^[1]

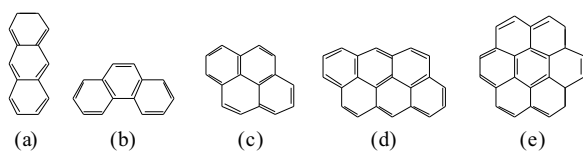


Figure 2: Examples of PAHs: (a) anthracene, (b) phenanthrene, (c) pyrene, (d) anthanthrene and (e) coronene.

Therefore, it is possible to change the periphery, size and shape of a PAH through substitution of both the ring atoms and their R groups resulting in various PAHs that exhibits unique properties which will be discussed below. PAHs have long been the focus of interdisciplinary research such as synthesis, characterisation, investigation of physical, chemical, biological and photophysical properties that render their applications in material and pharmaceutical sciences.^[3]

Properties of PAHs and their Importance

The early discoveries of the electrical and optoelectronic properties of PAHs have now led to promising applications in the field of organic electronics.^[4] The electrical and optoelectronic properties of such molecules rely heavily on extended π -conjugation. In this area, organic chemists have pursued various π -conjugation systems as active components for electronic and optoelectronic devices such as light-emitting diodes (LEDs), solar cells and many other molecular electronic devices.^[5] The key physical processes for these applications are the transport and recombination of electrical charges.

Particularly, the mobility of the charge carrier in the solid-state materials is one of the most important parameter that determines the device performance.^[6]

The thermal and chemical stabilities and the solubility of PAHs are further characteristic features which are essential for the processing of these materials. The thermal and chemical stabilities of PAHs depend not only on their size but also upon the topological arrangement of the benzenoid rings.^[4] Depending on their size and shape and the favourable overlap of π -orbitals in adjacent molecules these materials possess the ability to form ordered columnar mesophases with high charge carrier mobilities along the columnar axis. This makes them suitable as semiconducting materials.^[7] Hexa-*peri*-hexabenzocoronene (HBC) exhibits one of the highest intrinsic charge carrier mobilities for a discotic material.^[8]

The variation of the periphery, topology, size and shape of a HBC has a distinct impact on its electronic properties and its self-assembling behaviour and columnar superstructure.

Size

Increasing size leads to greater electron delocalisation and to a decreased difference between the HOMO and the lowest unoccupied molecular orbital (LUMO), which is readily visible in the colour of the material. For example when the HOMO and LUMO energy gap decreases, the emission maxima shift to the red region of the visible spectrum (Figure 3).^[7]

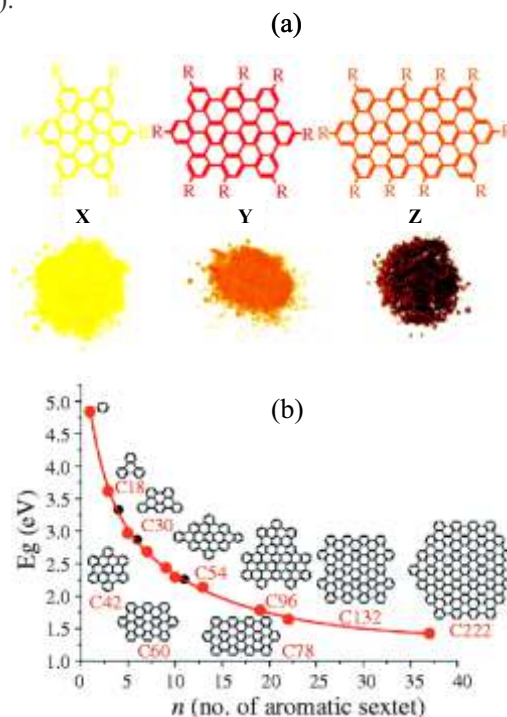


Figure 3: (a) Examples of PAHs (X, Y and Z) show the bathochromic shift of absorption with increasing size. (b) Correlation of the HOMO-LUMO bandgap versus the number of aromatic sextets.^[7]

Increasing the size of the core of a discotic material improves the order of the columnar superstructure. This is due to the large overlapping of π -surfaces and as a result their charge carrier mobility is enhanced. For example, moving from triphenylene (T), coronene mono-imide (CI), azocarboxylicimido-perylene (Per) to hexa-*peri*-hexa-benzocoronene (HBC) the charge carrier mobility increases with the increased size of the aromatic core (Figure 4 and Table 1).^[8]

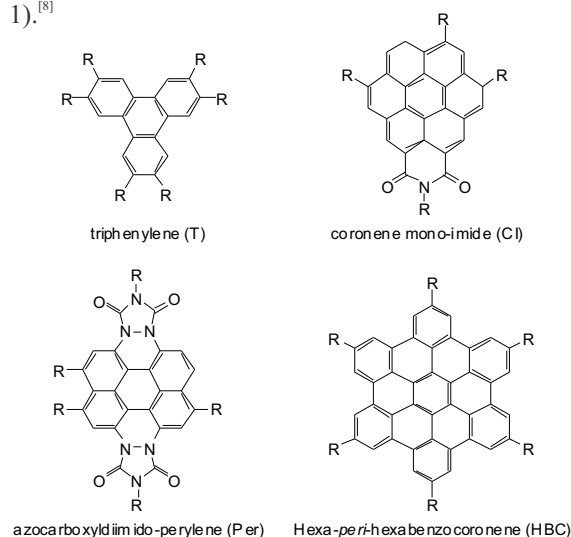


Figure 4: The molecular structures of the macrocycles forming the core of the discotic materials, R = alkyl chains.^[8]

Table 1: The intra-columnar charge mobilities ($\Sigma\mu_{ID}$) determined for a given macrocyclic core in the hexagonal columnar mesophase (D_h) and the crystalline solid phase (K) at temperatures just above and below the $K \rightarrow D_h$ transition temperature, respectively.^[8]

Core	Core size [n]	$\Sigma\mu_{ID}$ [$\text{cm}^2\text{V}^{-1}\text{s}^{-1}$] D_h phase (min-max)	$\Sigma\mu_{ID}$ [$\text{cm}^2\text{V}^{-1}\text{s}^{-1}$] K phase (max)
T	18	0.002-0.025	0.26
CI	29	0.24	0.24
Per	34	0.15-0.21	0.24
HBC	42	0.26-0.38	1.13

Shape

Another factor that affects the electronic properties of PAHs is shape and this is always correlated with the size. The versatility of the oxidative cyclodehydrogenation has led to the synthesis of large all-benzenoid hydrocarbons with different symmetries such as C_{2v} , C_3 and D_{6h} . PAHs up to a trimer with different geometries [i.e. trimer (a-b),^[4,7] triangle (c),^[9] diamond (d),^[4] linear (e)^[7] and ribbon (f-g)^[10] as shown in Figure 5 have been successfully synthesised by intermolecular oxidative cyclodehydrogenation of single HBC moieties or by intramolecular

cyclodehydrogenation of corresponding branched polyphenylenes.^[4] It has been predicted that polymer-HBC (e) and trimer-HBC (b) are also possible to stack in an ordered columnar which might allow charge carrier transport along HBC multicolumns (Figure 5).^[4]

Conjugated polymers (Figure 6) are also another set of architecture derived from PAHs. Polyphenylene-based polymers are one of the most important classes of conjugated materials for electronic applications such as light-emitting diodes (LED), solar cells or field-effect transistors (FET). These materials show blue-green emission in solution and with the increase of the planarity and the rigidity of the conjugated chains emission maxima shifts to red-region.^[7]

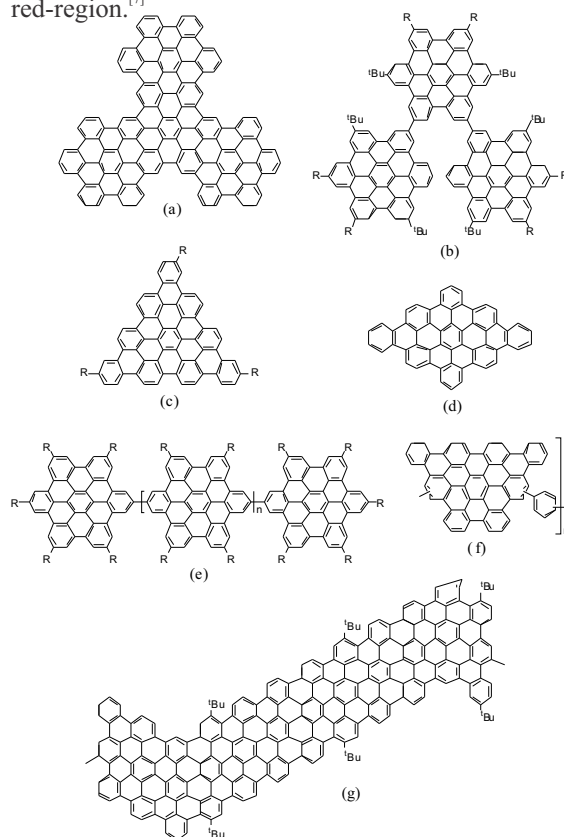


Figure 5: Representation of different shapes of HBCs: (a) Supracene trimer,^[4] (b) combined trimer-HBC,^[7] (c) triangle shape,^[9] (d) diamond shape,^[4] (e) combined linear-HBC^[7] and (f-g) ribbon shape.^[10]

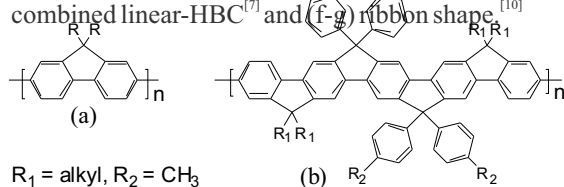


Figure 6: Polyphenylene-based conjugated polymers.^[7]

Substitution

As PAHs are large two-dimensional benzenoid structures their simplest form is when terminal carbon atoms (i.e. *ortho* and *para*) are substituted by hydrogen atoms ($R=H$). Generally PAHs with $R=H$ show extremely low solubility in most common organic solvents such as toluene, chloroform etc. This insolubility leads not only for problems when attempting to fully characterise them but also increases the difficulty of thin film or device fabrication.

Substituting these terminal hydrogens ($R=H$) with branched or *n*-alkyl groups leads to materials which are more soluble and assists the complete spectroscopic characterisation of these compounds. For example HBC (Figure 7 (a)) is very insoluble in common organic solvents. Therefore, it was necessary to grow the crystals of this material for structure determination from a pyrene melt.^[11] However, the *tert*-butyl substituted version of (a), Hexa-*tert*-butyl-hexa-*peri*-hexa benzocoronene (b) (Figure 7), is soluble in most common organic solvents. Crystals of (b) were obtained by slow evaporation in THF-pentane at room temperature.^[4]

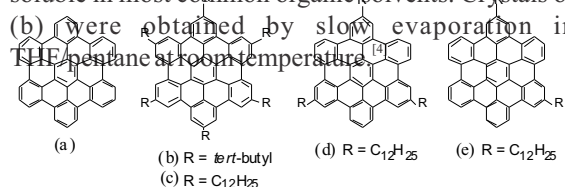


Figure 7: (a) Hexa-*peri*-hexabenzocoronene and (b-e) alkyl substituted hexa-*peri*-hexabenzocoronene.^[4,11]

Substitutions of the H atoms on HBCs with different types of alkyl groups i.e. $-C_{12}H_{25}$, $-OCH_3$, also influence the surface organisation and self-assembly.^[4,7] During the process of self-organisation, the disk-shaped molecules organise into columns that assemble into two-dimensional arrays, whereas the alkyl chains fill the intercolumnar space.^[12]

The HBCs properties can be modified through the architecture of the substituents, for example the alkyl chain length and the substitution disk corona.^[4] For instance, longer and more flexible side chains were expected to decrease the thermal phase transition. On the other hand, reducing the number of substituents and maintaining a high substitution symmetry of the disk-shaped building blocks such as compounds with D_3 symmetry (d), were shown to influence significantly their thermal and self-assembly behaviours compared to (e) (Figure 7).^[4,11]

Therefore, the purpose of substitution of the alkyl chains is to introduce solubility, processability, a rich thermotropic behaviour and their self-assembly in the solid state and at the solid-liquid interface.^[13]

Periphery

Tetracene (b), a constitutional isomer of

triphenylenes (a) (Figure 8), differs distinctly in its properties such as lower resonance energy, lower ionisation potential, small HOMO-LUMO gap and thermally far less stability.^[4] Dias^[14] zigzag and arm chair edge are two prominent periphery types that are observed in PAHs. For example HBCs contain an 'arm-chaired' periphery (Figure 8 (c)). When the 'arm-chaired' site of the HBC is modified to partial 'zigzag' peripheries (d-e) it was shown to lower the HOMO-LUMO gap (Figure 8). Indeed, the change of periphery and symmetry shows a pronounced influence on the electronic spectra.^[4] In addition, periphery also influences the self-assembly properties of the PAHs.

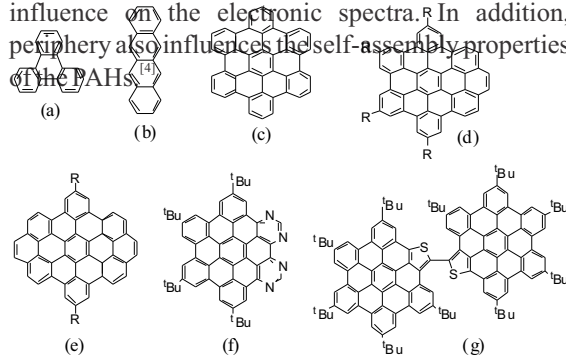


Figure 8: Series of PAHs: (a) triphenylene, (b) tetracene, (c) HBC 'arm-chaired' periphery, (d) and (e) HBC 'zigzag' periphery,^[7] (f) N-doped periphery (N-HSB)^[15] and (g) S-doped periphery (S-HSB).^[16]

Draper and Müllen among others have modified the periphery of the HBC by introducing heteroatoms, for example, nitrogen (f)^[15] and sulphur (g)^[16] (Figure 8). The systematic replacement of carbon atoms with electronegative nitrogen atoms enhances the electronic properties of the system because of the higher electron density.^[15] However, the inclusion of nitrogen donor atoms renders the HBC-type core overall electron-accepting. This confers on the new nitrogen-hetero superbenzenes (N-HSB)s (f) the dual advantage of ligand functionality and increased solubility (Figure 8).^[15]

All parameters discussed above intriguingly influence not only the materials' properties but also influence the careful molecular and supramolecular design required for optimum performance in electronic devices.

Many PAH systems have attracted attention in different areas of chemistry of late (e.g. polymer and material chemistry) due to their fascinating properties. Out of these different types of graphenes HBC has made a significant impact in this field for several reasons. These include its manageable size, shape and solubility which are desirable for the applications. This allows scientists to investigate their various characteristic properties in either the solid state or in solution using different techniques. The later property has been affected by the ability to alter

the atoms in the periphery and substitute the terminal H groups with functional groups such as alkyl and alkoxy groups. This allows HBCs to be studied in more detail than the highly insoluble large sheets and globular shaped PAHs which were synthesised from branched polyphenylenes.

Supramolecular Properties of Hexa-*peri* hexabenzocoronenes

PAHs undergo molecular self-assembly in the solid-state, generating supramolecular networks through π -stacking.^[4] HBCs are known to self-assemble into a columnar phase and may further organise into sheets which ultimately roll up like a carpet to form multi-walled nanotubes. The molecular self-assembly of HBC can be altered by substituents. For example, when HBC is functionalised with long-chain alkyl groups or alkoxy groups it assembles into columnar structures known as columnar liquid crystals. Columnar liquid crystals are characterised by their structural order and the manner in which the columns pack.^[4]

The solid state and the discotic liquid-crystal columnar packing arrangements change based on steric considerations. For example, when the periphery of the HBC core is substituted with 18 methoxy groups, the resulting compound permethoxylated hexa-*peri*-hexabenzocoronene (permethoxylated-HBC) (a) is sterically crowded (Figure 9). Therefore, the single-crystal structure of (a) displays a “double-concave aromatic core”. This molecule is arranged in a herringbone-type packing (b) and there is no dimer formation (inter-planar distance 13.05 Å).^[4] Whereas, the single-crystal structure of *tert*-butyl groups substituted HBC hexa-*tert*-butyl-hexa-*peri*-hexabenzocoronene (*tert*-butyl-HBC) (c) displays a planar but slightly bent aromatic core. *Tert*-butyl-HBC crystal structure shows the formation of dimers (inter-

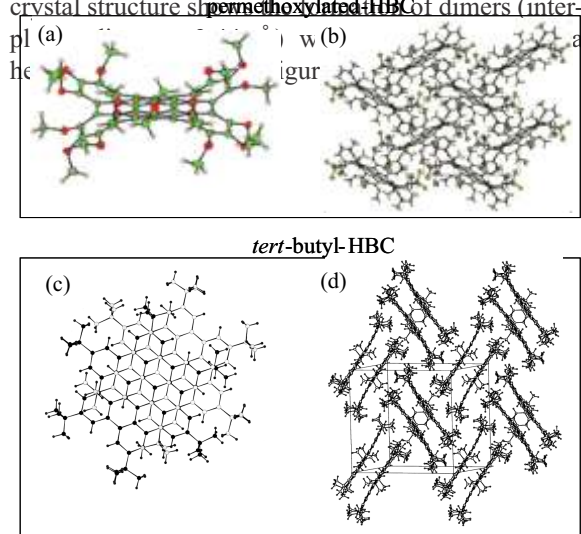


Figure 9: (a) The molecular structure of permethoxylated-HBC, (b) herringbone packing arrangement of permethoxylated-HBC, (c) the crystal structure of *tert*-butyl-HBC in dimeric projection and (d) herringbone packing arrangement of *tert*-butyl-HBC.^[4]

References

1. A. K. Geim, *Nat. Mater.* **2007**, 6, 183.
2. F. Munoz-Rojas, *Phys. Rev. B: Condens. Matter Mater. Phys.* **2008**, 77, 045301/1.
3. T. Henning, *Science* **1998**, 282, 2204.
4. K. Müllen, *Chem. Rev.* **2007**, 107, 718.
5. A. C. Grimsdale, *Chem. Rev.* **2009**, 109, 897.
6. A. Aleshin, A. J. Heeger, *Phys. Rev. B: Condens. Matter* **1997**, 56, 3659.
7. S. Mueller, K. Muellen, *Philos. Trans. R. Soc., A* **2007**, 365, 1453.
8. J. M. Warman, *Adv. Mater.* **2001**, 13, 130.
9. K. Müllen, *Angew. Chem.*, **2007**, 46, 3033.
10. A. G. Vitukhnovsky, *J. Lumin.* **2004**, 110, 232.
11. J. M. Robertson, *J. Chem. Soc.* **1961**, 1280.
12. D. Demus, *Handbook of Liquid Crystals, Volume 2B: Low Molecular Weight Liquid Crystals II*, **1998**.
13. K. S. Novoselov, *Nature* **2005**, 438, 197.
14. J. R. Dias, *J. Chem. Inf. Comput. Sci.* **2005**, 562.
15. S. M. Draper, D. J. Gregg, *J. Am. Chem. Soc.* **2002**, 124, 3486.
16. C. Martin, S. M. Draper, *Advances in Science and Technology* **2008**, 54., 120.



INTERNATIONAL CONFERENCE ON CHEMICAL SCIENCES (ICCS)
COLOMBO, SRI LANKA
20-22 June 2012

Theme:
Role of Chemistry Research in National Development

The Institute of Chemistry Ceylon is organizing an International Conference on Chemical Sciences, during 20-22 June 2012 at Waters Edge, Battaramulla and Sri Lanka Foundation Institute, Colombo, Sri Lanka.

The major aim of the conference will be to discuss how chemistry meets the global challenges of clean air, safe water, healthy food, dependable medicine from plants, and how the chemical education imparted to our students achieve the UN Millennium development goals.

The conference will, therefore, bring together chemists, environmentalists, food scientists, educationists and other scientists on a common platform to exchange ideas and discuss the role of chemistry research in national development.

The conference will, therefore, focus on the following main topics in chemistry. The names of the Chairpersons and the Secretaries/Co-ordinators of the topics are given below:

Topic	Chairperson	Secretary/Co-ordinator
Natural Products Chemistry	Professor Priyani Paranagama priyani@kln.ac.lk	Dr Vinitha Thadhani vinitha.ichemc@gmail.com
Food Sciences	Professor Siromi Samarasinghe siromi29@yahoo.com	Ms Dilini Gunawardena dilini_25@yahoo.com
Environmental Chemistry	Professor Oliver Ileperuma oliveri@pdn.ac.lk	Dr Sisira Weliwegama weliwegama@yahoo.com
Chemical Education	Professor J N O Fernando oleap@iname.com	Mrs K de S. Goonetilleke mnzoy@ou.ac.lk
New Technological Developments and Industrial Research	Dr Raj Parthipan parthiraj@gmail.com	Dr. Rathika Kandiah rkandiah@gmail.com

Abstracts on the above topics should be sent to the Secretary/Co-ordinator, identified above, for each topic.

Abstracts are also accepted in other main areas of chemistry and electronic copies in these areas should be sent by email to sotheeswaran@hotmail.com

Abstracts should be sent not later than 15 December 2011. Acceptance will be notified by 15 February 2012 to enable authors to pay the early bird Registration fees by 29 February 2012. Authors should indicate if they wish to present their papers orally or in the poster sessions.

The two best posters, in each of the above topics, will receive cash awards: First Prize - Rs 5,000 and Second Prize - Rs 3,000.

For more details visit the Institute websites: <http://www.ichemc.com/> or <http://www.ichemc.edu.lk/>

41st Annual Sessions of the Institute of Chemistry Ceylon 2012

Theme:

Role of Chemistry Research in National Development

Date: June, 2012

CALL FOR ABSTRACTS AND EXTENDED ABSTRACTS

Last Date for receiving abstracts and extended abstracts is **31st January 2012**

AWARDS 2012

The following awards will be presented at the Annual Sessions 2012 of the Institute of Chemistry Ceylon.

- **Dr. C L de Silva Gold Medal Award**

Awarded for an outstanding research contribution in any branch of Chemical Sciences and/ or the use of such research for National Development during the last five (5) years in Sri Lanka. Credit will be given for the utilization of local raw materials, and where the contribution has already resulted in (i) a publication in a Citation Indexed Journal or (ii) Registering a Patent or (iii) where the contribution has already resulted in a positive impact in the development and innovation in the industry.

- **INSTITUTE OF CHEMISTRY SILVER MEDALS**

Devanathan Memorial Award

Awarded for an exceptional research contribution of an original nature in the field of Physical Chemistry and or related areas, such as Physical-Inorganic, Physical-Organic and Biophysical chemistry.

Chandrasena Memorial Award

Awarded for an exceptional research contribution of an original nature in the field of Organic Chemistry and / or related areas such as Biochemistry, Pharmacognosy, Molecular Biology and Bioactivity studies.

Ramakrishna Memorial Award

Awarded for an exceptional research contribution of an original nature in the field of Inorganic and/ or Analytical Chemistry and/or related areas such as Bio-inorganic Chemistry or Bio- analytical Chemistry.

- **INSTITUTE OF CHEMISTRY BRONZE MEDALS**

Kandiah Memorial Awards

Awarded for the best research contribution in Chemistry carried out by a postgraduate student registered for a postgraduate degree by either course work or/ and research at a Higher Educational Institute in Sri Lanka and for work carried out in Sri Lanka, with the exception of special analysis that cannot be done in the country. Such results should be less than 20% of the findings from the work. Sandwich programs carried out partially abroad do not qualify for the award.

Kandiah Award for Basic Chemistry

For research predominately in basic Chemistry (Organic, Inorganic, Physical, and Analytical).

Kandiah Award for Applied Chemistry

For research in Chemistry related areas such as polymer, food, biochemistry, biotechnology, where interdisciplinary research is involved and provided that chemistry has a central role and comprises at least 50% of the content.

Kandiah Memorial Graduateship Award

For the best piece of research in the Chemical Sciences carried out by a Graduate Chemist of the College of Chemical Sciences/ Institute Chemistry Ceylon registered with a Higher Education Institute for a Post Graduate Degree.

- **Professor M. U. S. Sultanbawa Award for Research in Chemistry**

Awarded for the best research paper presented at the Annual Sessions of the Institute of Chemistry Ceylon, for work carried out and completed in Sri Lanka.

Closing date for receiving applications/ nominations for the above awards: **31st December 2011**

Further information could be obtained from the Registrar, Institute of Chemistry Ceylon or www.ichemc.edu.lk

Report on the 40th Annual Sessions & 70th Anniversary Celebrations

The 40th (fortieth) Annual Sessions of the Institute of Chemistry, Ceylon was held from 16th to 18th June 2011 on the theme “Chemistry education for the Wellbeing of Society”.

1. Ceremonial Inauguration

The Ceremonial Inauguration was held at the Sri Lanka Foundation Institute (SLFI), Colombo 7 on 16th June 2011 from 8.00 a.m to 11.10 a.m. The Chief Guest at the event was Professor J. A. Pincock of the Department of Chemistry, Dalhousie University, Canada.

The proceedings began, as is traditional, with the lighting of the oil lamp followed by the National Anthem. The “Welcome Address” was delivered by Professor M. D. P De Costa, President, Institute of Chemistry Ceylon. Professor M. D. P De Costa, then, delivered his Presidential address on “Chemistry and Society”. This was followed by the Chief Guest's address on “Better living through Chemistry” which was very informative. The Guest of Honour Mr Chandima Perera, Head of Beverages, John Keells Ltd gave a presented an advertisement on the method of extraction of ginger for the preparation of EGB.

This was followed by distribution of awards and certificates.

The Chief Guest together with the Guest of Honour distributed the following Awards, Prizes and Certificates:

- § Distinguished Services Award : Professor (Mrs) Sujatha Hewage
- § Institute of Chemistry Gold Medal: Mr N M S Hettigedera
- § Long Service Award: Ms Anoma Wijesuriya
- § Graduateship Examinations in Chemistry, Scholarships, Prizes and Award
- § Winners at the All Island Interschool Chemistry Quiz Contest

An invited speech titled “From rocks to community health – Tracing the chemical pathways of an element” was delivered by Professor C B Dissanayake, Director, IFS, Kandy.

Professor Sotheeswaran, President elect, proposed the vote of thanks.

2. Annual General Meeting

The 40th Annual General Meeting of the Institute of Chemistry was held at 12.00 noon on Wednesday 16th June 2011 at the SLFI Auditorium, with Professor M D P De Costa in the chair. About 75 members were present. The minutes of the 39th Annual General

Meeting were adopted. The audited financial Statements for 2010 were approved. The election of the office bearers and members of the Council for the year 2011/2012 followed. The AGM concluded with the members present being invited for lunch.

3. Theme Seminar - “Photochemistry for the well being of society”.

Theme Seminar was held on the second day of the annual sessions, Thursday 17th June 2011 from 9.00 am to 4.30 pm at the SLFI. Presentations were made by Professor M D P De Costa, Professor J A Pincock, Professor O A Illeperuma, Mr. Asanga Ranasinghe, Dr. R Senthilnithy, Professor Pradeep Jayaweera, Dr. Ranil de Silva, Professor Nalin de Silva and Professor K R R Mahanama on a variety of photochemistry related topics. Presentations were followed by a discussion. Theme seminar was a very successful event. Majority of the participants were students of the College of Chemical Sciences.

4. Technical Sessions

The technical sessions were held on Wednesday 16th June 2011 afternoon at the SLFI and Saturday 18th June 2011 morning at the “Adamantane House”. Seventeen research papers on current research work carried out were presented.

5. Annual Dinner & Induction of the New President

The Annual Dinner & Induction of Prof. S Sotheeswaran, the new President of ICHEMC, was held on 16th June 2011 at Grand Ballroom, Galle Face Hotel. The Chief Guest for the event was Professor (Mrs) Sujatha Hewage. The guest of honour was Dr. K D P Hemalal.

6. Sponsorships & Donations

Unilever Sri Lanka Ltd, John Keells Holdings PLC, Hemas Manufacturing (Pte) Ltd, Techno Instruments (Pvt) Ltd, Fonterra Brands Lanka (Pvt) Ltd, Antler Fabric Printer Ltd, CIC Holdings PLC, Glaxowellcome Cey Ltd, Haycarb PLC, Holcim Lanka Ltd, K M J Laboratories, LionLabs, Microchem Laboratories (Pvt) Ltd, SPMC, Sugarcane Research Institute, Graduate Chemists and many more donations.

M. R. M. Haniffa & M N K De S Goonetillake
Hony. Joint Secretaries

PUBLICATIONS OF THE INSTITUTE OF CHEMISTRY CEYLON

Monograph	Title	Author	Price
01	Textile Fibers	Mr T Rajasekeram	Rs.50/-
02	Principles of Food Preservation	Prof U Samarajeewa	Rs.75/-
03	Biotechnology	Prof C P D W Mathew	Rs.75/-
04	Recombinant DNA Technology	Prof J Welihinda	Rs.75/-
05	Natural Toxins in Foodstuffs	Prof E R Jansz & Ms A S Perera	Rs.50/-
06	Fat Soluble Vitamins	Prof E R Jansz & Ms S Malavidana	Rs.50/-
07	Nucleic Acid and Protein Synthesis	Prof J Welihinda	Rs.75/-
08	Extraction of Energy from Food	Prof J Welihinda	Rs.50/-
09	Corrosion of Materials	Dr A M M Amirudeen	Rs.75/-
10	Vitamin C-Have all its mysteries been Unravalled ?	Prof E R Jansz & Ms S T C Mahavithanage	Rs.75/-
11	*Environmental Organic Chemistry (second edition)	Prof S Sotheeswaran	Rs.150/- (US \$3)
12	Enzyme Kinetics and Catalysis	Prof (Mrs) S A Deraniyagala	Rs.100/-
13	Insecticides	Prof (Mrs) Sukumal Wimalasena	Rs.95/-
14	Organotransition Metal Catalysts	Dr S P Deraniyagala & Dr M D P De Costa	Rs.75/-
15	Some Important Aspects of Polymer Characterization	Dr L Karunanayake	Rs.75/-
16	Hard & Soft Acids & Bases	Prof (Mrs) Janitha A Liyanage	Rs.65/-
17	Chemistry of Metallocenes	Dr Sarath D Perera	Rs.65/-
18	Lasers	Dr P P M Jayaweera	Rs.65/-
19	*Life and Metals	Prof (Mrs) Janitha A Liyanage	Rs.75/-
21	*Silicones	Prof Sudantha Liyanage	Rs.65/-
22	Pericyclic Reactions: Theory and Applications	Dr M D P De Costa	Rs.65/-
23	Inorganic NMR Spectroscopy	Prof K S D Perera	Rs.65/-
24	Industrial Polymers	Dr L Karunanayake	Rs.75/-
25	NMR Spectroscopy	Dr (Mrs) D T U Abeytunga	Rs.65/-
26	Mosquito Coils and Consumer	Ms D K Galpoththage	Rs.100/-
27	Atomic Absorption Spectrometry	Dr K A S Pathiratne	Rs.100/-
28	Iron Management on Biological Systems	Dr (Ms) R D Wijesekera	Rs.100/-
29	Nutritional Antioxidants	Prof. (Mrs) Sukumal Wimalasena	Rs.100/-
30	*f-Block Elements	Prof Sudantha Liyanage	Rs.65/-

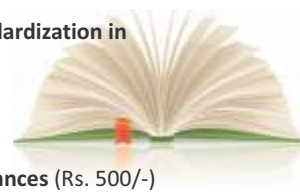
* - Second Edition /new print published on popular demand

CCS Publications

01	Functional Group Analysis in Organic Chemistry	Prof AAL Gunatilake	Rs. 175/-
02	Zinc Metalloproteins	Prof S Sotheeswaran Prof (Ms) R D Wijesekera	Rs. 175/-

General Publications

- ★ **Chemist & The Environment** (Rs.300/-)
- ★ **Infrastructure Support Services for Industrial Development** (Rs.200/-)
- ★ **Chemical Industries in Sri Lanka – Part II** (Members: Rs. 200/-, Non-members: Rs.275/-)
- ★ **Proceedings of the Workshop on the Technological aspects of the Production & Processing of Essential oils in Sri Lanka** (Rs.100/-)
- ★ **Proceedings of the Training Seminar on Towards a Cleaner Industrial Environment in the New Millennium** (Rs.150/-)
- ★ **A-Level Chemistry Facts, Patterns & Principles by Dr. Seetha I Rodrigo** (Rs.1500/-)
- ★ **Proceedings of the Prof R S Ramakrishna Memorial Training Seminar on Modern Analytical Methods**(Rs.200/-)
- ★ **Historical Accounts of the Educational Activities (1972 - 2004)** (Rs.350/-)
- ★ **Proceedings of the Training Seminar cum Workshop on Sampling, Statistics and Standardization in Chemical Analysis and Environmental Management** (Rs.150/-)
- ★ **Polymer Industries of Sri Lanka** (Rs. 200/-)
- ★ **Industry & Environment** (Rs. 200/-)
- ★ **Herbal Medicine Phytopharmaceuticals and Other Natural Products: Trends and Advances** (Rs. 500/-)
- ★ **Chemistry in Sri Lanka** (Rs. 150/-)





RSC NEWS

THE ROYAL SOCIETY OF CHEMISTRY SRI LANKA SECTION

1. Membership

According to the records sent to us from the parent body, a breakdown of the membership is as follows:-

Category	Abbreviation	Number
Fellow Life Member.	F E L	05
Fellow C Chem.	F C C	09
Member	M E M	26
Associate Member	A M E	12
Affiliate Member	A F F	01
Affiliate /Under Graduate. A F U		<u>02</u>
Total Membership as at March 2011		<u>55</u>

2. Committee of Management

The following were elected to the Committee at the 50th Annual General Meeting held on 15th July 2011.

Chairman	- Prof. Sudantha Liyanage
Vice Chairman	- Mr. W J P D Jayalath
Chairman Elect	- Dr. M P Deeyamulla
Hony. Secretary	- Mr. I M S Herath
Hony. Treasurer	- Prof. W S Fernando
Committee Members -	Dr. Positha Premaratne
	Mr. W A P Silva
	Mr. S Perasiriyana
	Mr. R M G B Rajanayake
	Prof. L G Chandrasena
	Mr. Sulith Liyanage

3. Committee Meetings

There were 12 Committee Meetings held during the period, July 2010 to July 2011. The venue of these meetings was the office of the Royal Society of Chemistry SL Section at the S L A A S Headquarters. These meetings were held to discuss the R S C SL Section's, new plans and strategies with regard to organizing the activities for the year 2010/2011 and thereafter.

4. Activities

4.1 Contributions to Activities of the Institute of Chemistry Ceylon

(a) Full page advertisement of "Chemistry in Sri Lanka".

(b) Annual Dinner

(c) Award for the Best Performance at the Graduate ship Examination in Chemistry Part II Theory Examination

(d) Contributions for the International Conference

4.2 All - Island Inter School Chemistry Essay Competition.

4.3 Inter - University Chemistry Competition.

4.4 Teacher training program.

4.5 Advanced Level chemistry seminar.

4.6 Donation of teaching and learning resources for Chemical Society of selected University.

4.7 Book donation program.

4.8 Popular Lectures.

4.9 Industrial Visit.

4.10 Writing Monographs by few committee members.

4.11 Newton A. Dias Weerasinha Memorial Scholarship 2011/2012

5. Web Site

The members are reminded of the web site of our Section, the address of which is as follows:-

[www.rsc.org/Membership/Networking/InternationalSections/Sri Lanka/ index. asp](http://www.rsc.org/Membership/Networking/InternationalSections/SriLanka/index.asp).

I M S Herath
Hony Secretary